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The GeoPEARL model
Part II. User guide and model description update

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Het rapport in het kort

Nederland heeft sinds kort een nieuwe beslisboom om het risico van uitspoeling van bestrijdingsmiddelen naar het grondwater te kunnen beoordelen. In deze beslisboom wordt beoordeeld of de concentratie van bestrijdingsmiddelen in het grondwater de EU drinkwaternorm van 0,1 μg/L zal overschrijden. De nieuwe beslisboom houdt expliciet rekening met het oppervlak waarop het middel wordt toegepast. Een middel kan uitsluitend worden toegelaten indien de concentratie in het grondwater over een lange periode lager is dan 0,1 μg/L, onder tenminste 90% van het oppervlak waarop het middel zal worden verbruikt. Om dit criterium te kunnen toetsen is het model GeoPEARL ontwikkeld. Dit model zal een centrale rol gaan spelen in het nieuwe toelatingsbeleid. Dit rapport bevat een handleiding van het model, met nadruk op de nieuwe registratieprocedure. Het rapport dient te worden gebruikt in combinatie met rapport 601450019, dat de nieuwe beslisboom beschrijft.

Trefwoorden: bestrijdingsmiddelen; registratie; uitspoeling; modellering; GeoPEARL; handleiding

Abstract

Recently, the Netherlands has adopted a new decision tree for evaluating the leaching potential of pesticides, specifically to see if the concentration in groundwater exceeds the EU drinking-water limit of 0.1 µg/L. The spatial criterion in the new decision tree states that the long-term average concentration of a pesticide or its relevant metabolites should not exceed the drinking-water limit for at least 90% of the surface area where the pesticide is potentially used. A spatially distributed model, 'GeoPEARL', has been developed to scientifically test the above criterion. GeoPEARL will play a key role in the new Dutch decision tree. The aim of this report is to provide a guideline on the use of GeoPEARL, with special emphasis on the Dutch registration procedure. This report should be used in combination with RIVM report no. 601450019, which describes the new decision tree and the role of GeoPEARL in this tree. Background information, including the theory behind the model, can be found in the earlier RIVM report, no. 716601007.

Keywords: pesticides; registration; leaching; modelling; GeoPEARL; manual

Preface

Pesticide behavior in soils and leaching to the groundwater has widespread attention of the Dutch Ministries of VROM (Ministry of Spatial planning, Housing and the Environment) and LNV (Ministry of Agriculture, Nature and Food Quality). For this reason, they commissioned RIVM and Alterra to develop methods and tools to be used in the evaluation of pesticide registration and to assess the overall environmental quality with respect to pesticides. Since 1987, RIVM and Alterra have co-operated in several projects to serve the goals of the ministries with regard to pesticide policy. Particularly in the field of pesticide leaching this long-term co-operation has led to products that are not only used for the Dutch registration procedure, but in international context as well.

GeoPEARL, the tool described in this report, will play a central role in the new Dutch decision tree for evaluating the leaching behavior of pesticides in the Dutch registration procedure. During the periode 2002-2003, beta versions of GeoPEARL were presented to stakeholders in the field of pesticide registration. Discussions with stakeholders have triggered some model modifications. Also, the PEARL team has developed the GeoPEARL User Interface, which gives easy access to data and model. With the release of this model version, GeoPEARL becomes accessible to a broad public.

GeoPEARL makes use of results obtained in related projects. The spatial schematisation was created within the framework of the STONE project, a co-operation of Alterra, RIZA and RIVM. The PEARL team acknowledges the participants to the stakeholder meetings for stimulating discussions and suggestions for improvements. The group consisted of the following individuals (alphabetical order):
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Samenvatting

Nederland heeft sinds 1988 gebruik gemaakt van een beslisboom om het risico van uitspoeling naar het grondwater te kunnen beoordelen. Door recente ontwikkelingen op EU-niveau was het noodzakelijk om deze beslisboom te herzien om de afstemming met de EU optimaal te houden. Uitgangspunt is het EU-standpunt dat het grondwater bescherming behoeft. De EU-invulling van deze bescherming geeft aan dat de concentraties van individuele werkzame stoffen en relevante metabolieten in het grondwater niet hoger mogen zijn dan 0,1 μg/L. Om te kunnen functioneren in een beslisboom is echter een meer operationele en toetsbare norm nodig. De nieuwe beslisboom geeft als operationeel criterium dat de concentratie in het grondwater over een lange periode (20 jaar) lager moet zijn dan 0,1 μg/L, onder tenminste 90% van het oppervlak waarop de stof wordt gebruikt.

De nieuwe beslisboom bevat dus, in tegenstelling tot de vroegere procedure, een expliciet ruimtelijk criterium. Om dit criterium wetenschappelijk te kunnen toetsen is een ruimtelijk verdeeld uitspoelingsmodel, GeoPEARL, ontwikkeld. GeoPEARL berekent de uitspoeling van een stof specifiek voor het toedieningsareaal van de stof.

Dit rapport bevat een handleiding van het model, waarbij de nadruk ligt op toepassing in het kader van de nieuwe Nederlandse registratieprocedure. Dit rapport dient gebruikt te worden in combinatie met RIVM rapport 601450019, waarin zowel de nieuwe beslisboom als de rol van GeoPEARL in deze beslisboom, beschreven worden. Achtergrondinformatie over het model zelf, inclusief de theorie, zijn te vinden in een eerder verschenen RIVM rapport, namelijk rapport 716601007.

GeoPEARL bestaat uit verschillende componenten, waaronder het rekenhart (de ‘kernel’) en een grafische gebruikersinterface (GUI). Het model kan zowel met als zonder GUI worden gebruikt; het rapport beschrijft beide mogelijkheden.

Het eerste deel van het rapport beschrijft stap voor stap hoe het model via de GUI dient te worden gebruikt. De GUI is zodanig opgezet dat standaardtoepassingen ten behoeve van de toelatingsprocedure gemakkelijk kunnen worden uitgevoerd. De GUI geeft toegang tot de benodigde data, genereert invoerbestanden voor het rekenhart, voert de berekeningen uit en genereert rapporten en kaarten. De gegenereerde kaarten en rapporten kunnen direct gebruikt worden in een toelatingsdossier. De meeste gebruikers zullen het model via de GUI benaderen.

Het tweede deel van het rapport gaat in op het gebruik van de het model zonder de GUI. Gebruik van het model zonder GUI biedt een aantal extra mogelijkheden. Zo is het mogelijk een andere ruimtelijke schematisatie in te voeren en is toepassing van het model op een grid mogelijk. Toepassingen zonder de GUI vergen echter meer kennis van de gebruiker. Deze versie is daarom uitsluitend geschikt voor gebruikers die vertrouwd zijn met toepassing van complexe numerieke modellen.

Summary

Recently, the Netherlands have adopted a new decision tree for the evaluation of the leaching potential of pesticides. In this decision tree, it is evaluated whether the concentration in groundwater exceeds the EU drinking water limit, which is 0.1 µg/L. The new decision tree contains a spatial criterion: the long-term average concentration of a pesticide or its relevant metabolites should not exceed the drinking water limit across at least 90% of the area of use of the pesticide. To scientifically test the above spatial criterion, a spatially distributed pesticide leaching model, referred to as 'GeoPEARL', has been developed. GeoPEARL calculates the leaching of a pesticide and its metabolites to the uppermost groundwater for the area of use. The most important result for the Dutch pesticide registration procedure is the 90th areal percentile of the median leaching concentration over a period of 20 years. This report gives a guidance on the use of GeoPEARL, with special emphasis on the Dutch registration procedure. It should be used in combination with RIVM report 601450019, which describes the new decision tree and the role of GeoPEARL in this new decision tree. Background information on GeoPEARL, including theory, can be found in the earlier RIVM report 716601007.

GeoPEARL consists of a computation kernel and a Graphical User Interface. The model can be used with or without the Graphical User Interface. The manual describes both routes. For standard applications, both model versions will give the same results.

The first part of the manual gives a stepwise description of the Graphical User Interface. The Graphical User Interface is set-up to facilitate the Dutch registration procedure; summary reports generated by the Graphical User Interface can directly be used in a registration dossier. The GUI gives easy access to the most important components of GeoPEARL, like the generation of input files, model execution, output processing and generation of reports and maps. For most modelers, this part of the manual will be sufficient.

The second part of the manual describes how the model can be used without the graphical user interface. When the model is applied in this way, the user will have more possibilities. It is for example possible to import a different spatial schematisation or run the model on a grid. The command-line version, however, is also more difficult to use. This version should therefore only be used by those modelers that are familiar with complex numerical simulation models.

1 Introduction

Recently, the Netherlands have adopted a new decision tree for the evaluation of the leaching potential of pesticides. In this decision tree, it is evaluated whether the concentration in groundwater exceeds the EU drinking water limit, which is 0.1 µg/L. The new decision tree contains a spatial criterion: the long-term average concentration of a pesticide or its relevant metabolites should not exceed the drinking water limit across at least 90% of the area of use of the pesticide. To scientifically test the above spatial criterion, a spatially distributed pesticide leaching model, referred to as 'GeoPEARL', has been developed. GeoPEARL calculates the leaching of a pesticide and its metabolites to the uppermost groundwater for the area of use. The most important result for the Dutch pesticide registration procedure is the 90th areal percentile of the median leaching concentration over a period of 20 years. Further background information on the new decision tree on leaching can be found in RIVM report 601450019 (Van der Linden *et al.*, 2004).

This report contains a user-manual of GeoPEARL 1.1.1., with special emphasis on the Dutch registration procedure. Background information on GeoPEARL, including the theory, can be found in the earlier RIVM report 716601007 (Tiktak *et al*., 2003). In some parts of this document, reference is also made to the manual of FOCUS PEARL 1.1.1. (Tiktak *et al.*, 2000). This pertains particularly to the guidance on the derivation of pesticide properties. It is therefore essential that both documents are available. All documents are available at the RIVM website (http://www.rivm.nl) and the PEARL website (http://www.pearl.alterra.nl).

The manual consists of two parts. In section 2, the Graphical User Interface is described. The Graphical User Interface gives easy access to the most important components of GeoPEARL, like the generation of input files, model execution, output processing and generation of the most important output maps and tables. Most users will use the GUI version of GeoPEARL only.

Section 3 contains a description of the command line version of GeoPEARL. The command line version of GeoPEARL is more flexible, but is also more difficult to use. Reasons to use the command line version of GeoPEARL may be:

- implementation of GeoPEARL on a grid computing system;
- import of a different spatial schematization, so that the model can be used for other countries.

The command-line version of GeoPEARL should only be used by experienced modelers. In contrast to the GUI version, the user can change all model inputs and this can more easily give rise to errors.

Section 4 and section 5 contain updates of the theory.

Background documentation to be used in combination with the manual

1. *The FOCUS PEARL Manual:* Tiktak, A., F. van den Berg, J.J.T.I Boesten, M. Leistra, A.M.A. van der Linden and D. van Kraalingen. 2000. Pesticide Emission Assessment at Regional and Local Scales: User Manual of FOCUS PEARL version 1.1.1. RIVM report 711401008, RIVM, Bilthoven, the Netherlands.
2. *The GeoPEARL background document:* Tiktak, A., A.M.A. van der Linden and J.J.T.I. Boesten. 2003. The GeoPEARL model. Model description, applications and manual. RIVM report 716601007, RIVM, Bilthoven, the Netherlands.
3. *Scientific publication on GeoPEARL:* Tiktak, A., D.S. de Nie, A.M.A. van der Linden and R. Kruijne. 2002. Modelling the leaching and drainage of pesticides in the Netherlands: The GeoPEARL model. Agronomie (22):373-387.
4. *The new decision tree on leaching:* Van der Linden, A.M.A., J.J.T.I. Boesten, A.A. Cornelese, R. Kruijne, M. Leistra, J.B.H.J. Linders, J.W. Pol, A. Tiktak and A.J. Verschoor. 2004. New decision tree for the evaluation of pesticide leaching from soil. RIVM report 601450019, RIVM, Bilthoven, the Netherlands.

2 User's guide of the GeoPEARL User Interface

This chapter gives an overview of the GeoPEARL user interface, which is an integrated environment for data storage and data retrieval, model control and viewing the output data (Figure 1). The user communicates with the GeoPEARL modeling system through the graphical user interface. This interface is linked with a relational database. It also generates the input files for the GeoPEARL executable. GeoPEARL in its turn calls the PEARL model. It does so for each unique combination of soil type, climate district, etc. These unique combinations are called *plots*. The output of GeoPEARL is transferred back to the user interface, from where it is stored in the database.

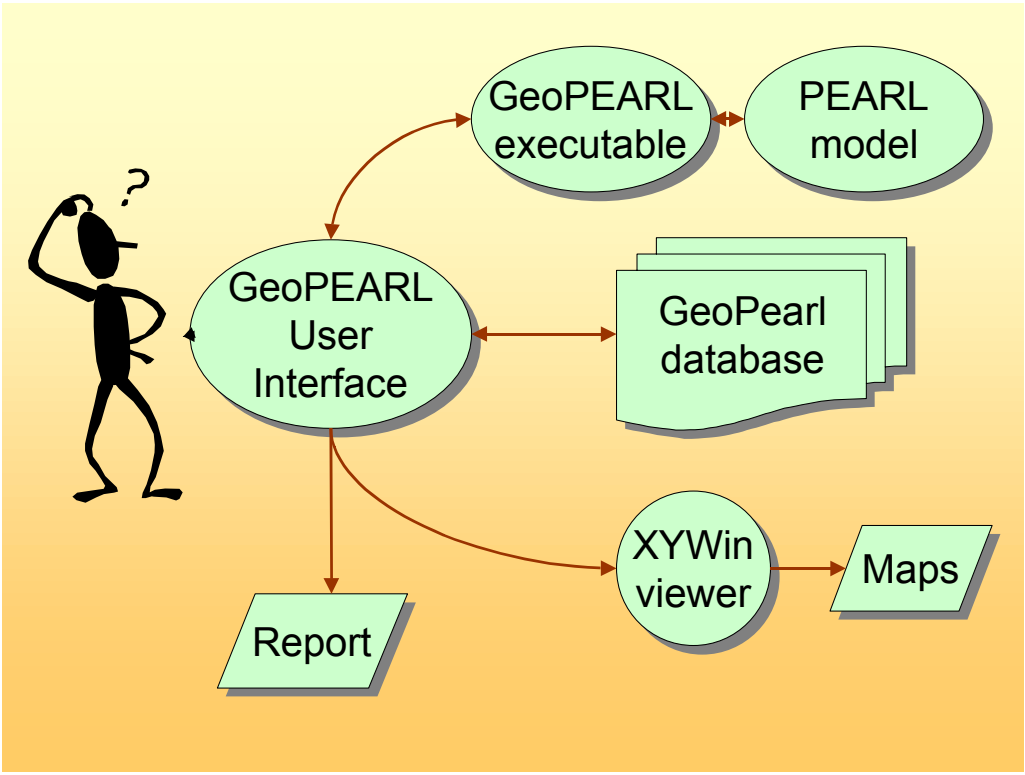

Figure 1. Overview of the GeoPEARL modeling system.

With the user interface, the following tasks can be carried out:

- organize and edit substance and application data;
- access the standardized model runs, which should be used for the Dutch pesticide registration procedure;
- control the model;
- view maps of major input variables;
- run the model;
- display a summary report, containing percentiles of the leaching concentration;
- display output maps;
- generate graphics files, which can be imported in (for example) Word.

2.1 Database structure

In order to organize the data efficiently, the data are stored in a relational database. Figure 2 shows how the data are organized in this database. Notice that the structure of the database has much in common with the structure of the FOCUS PEARL database (see Tiktak *et al.*, 2000 figure 19). As shown in later sections of this manual, the screens of the GeoPEARL GUI have the same set-up as the database.

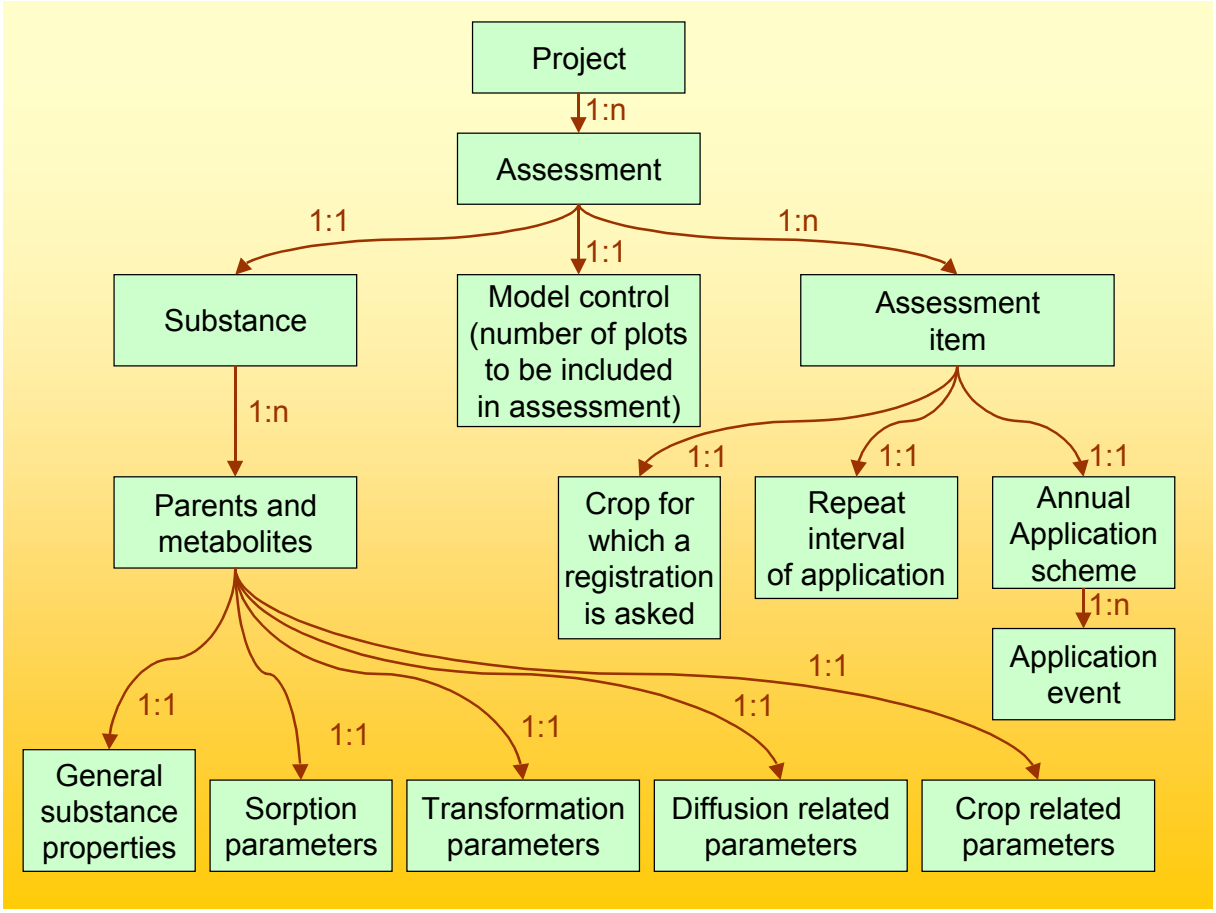

Figure 2.Overview of the GeoPEARL database. Only parameters that can be changed by the user are included in the diagram.

Like the FOCUS PEARL database, the GeoPEARL database has a hierarchy. The highest level of the database is the *project level*. Here, the user can group several assessments, based on a common criterion (e.g. all assessments related to a particular registration dossier). The second highest level is the *assessment level*. An assessment is the basic entity in GeoPEARL. A GeoPEARL assessment is carried out for a single substance, but may consist of several so-called *assessment items*. Assessment items are combinations of a crop for which a registration is asked and an application scheme. This implies that different crops can have different application schemes.

The GeoPEARL database also contains the data of the spatial schematization, such as soil type, climate district and drainage system. These data are locked and cannot be changed by the user; for this reason they are not shown in figure 2.

Assessments versus assessment items
Assessments are the central entity in the GeoPEARL GUI. For each assessment, the GUI calculates the area of usage and summary statistics like the 90th percentile of the leaching concentration at the area of usage, the latter being the target variable in the Dutch registration procedure (see Tiktak *et al.*, 2003, page 28). As mentioned above, an assessment can consist of various items. For example, a company might wish to request a registration for maize, potatoes and cereals. In that case, the assessment must contains three items. For each item, a GeoPEARL run is carried out and the 90th percentile of the leaching concentration is calculated for the total area of maize, potatoes and cereals.

2.2 Installation of the GeoPEARL User Interface

Before using GeoPEARL, you have to install the model. The model comes in a self-extracting archive, called geopearl_1_1_1.exe. This archive is available at the download page of the PEARL website, which is at the address http://www.pearl.alterra.nl. The size of this archive is approximately 150 Mbytes, so you need a fast internet connection for downloading (ADSL or better). The very first step of the installation procedure is to run the GeoPEARL self extractor application (figure 3). Running this application will automatically install the installation files to a directory of your choice (to be specified in the dialog 'destination folder'). It is advised to archive the installation files, as these may later be required to remove GeoPEARL.

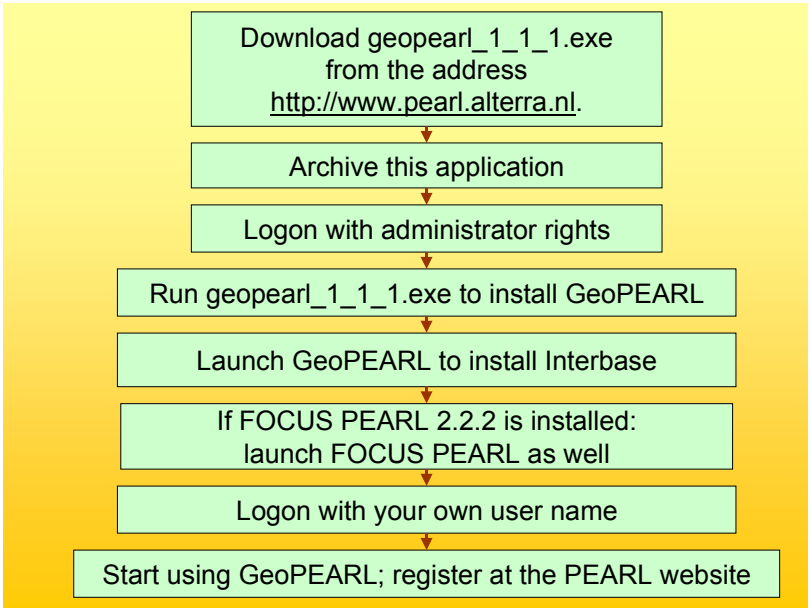
Download geopearl_1_1_1.exe from the address http://www.pearl.alterra.nl.
Archive this application
Logon with administrator rights
Run geopearl_1_1_1.exe to install GeoPEARL
Launch GeoPEARL to install Interbase
If FOCUS PEARL 2.2.2 is installed: launch FOCUS PEARL as well
Logon with your own user name
Start using GeoPEARL; register at the PEARL website

Figure 3. Installation procedure of GeoPEARL 1.1.1.

During the setup procedure, you will see the license agreement and the contents of the file ReadmeDuringInstallation.rtf. We strongly recommend reading the information in these files; particularly if you already have a GeoPEARL database, it is important that you read the instructions. They can be found back in the GeoPEARL directory. You should at least be aware of the following:

– the operation system must be Windows NT4 or higher. Windows 95 and Windows 98 are no longer supported by the PEARL team.

- you must have full administration rights during the installation procedure *and during the first time that you start using GeoPEARL*. If you don't have full administration rights, logon to your computer with a user name that has administrator rights. It may be necessary to contact your systems operator.
- if a FOCUS PEARL 2.2.2. installation is present at your computer, start FOCUS PEARL with administration rights to restore the connection with Interbase. If you don't do this, FOCUS PEARL will not start anymore.

Deployment licenses
GeoPEARL and FOCUS PEARL 2.2.2. both use an InterBase database. The use of this database requires the installation of a database engine, the so-called InterBase server. Each user must have a so-called *deployment license* for using this software. This deployment license can be obtained free of charge from Alterra. You need only one deployment license for GeoPEARL and FOCUS PEARL. *Only registered users can get a deployment license, so please register at the PEARL website.*

2.3 Getting started with the GeoPEARL User Interface

As in FOCUS PEARL, the user should first define the building-blocks of an assessment (see figure 2). This implies that first the substances and application schemes must be defined. This comes down to the following steps (figure 4):

1. Define or edit substances. Physico-chemical properties, sorption parameters, transformation parameters and parameters for interaction with plants should be defined for the substance and all its metabolites to be included in the calculations.
2. Define or edit the application schemes. As each assessment item may have its own application scheme, several assessment schemes may be required (see section 2.1).

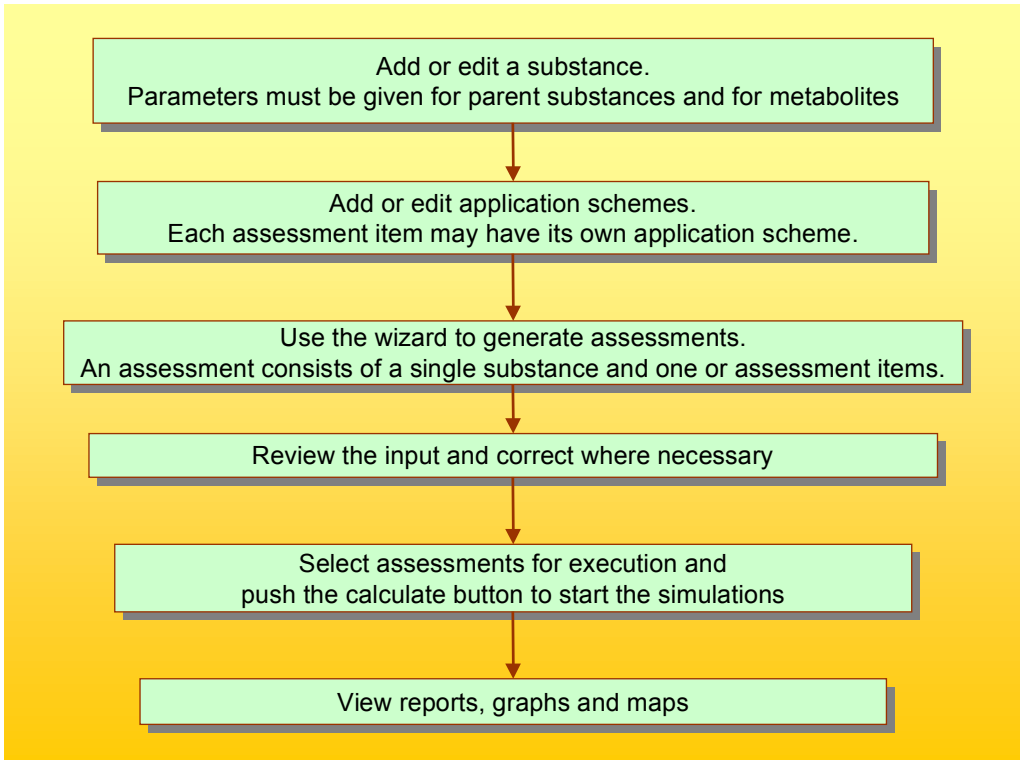
Add or edit a substance.
Parameters must be given for parent substances and for metabolites
Add or edit application schemes.
Each assessment item may have its own application scheme.
Use the wizard to generate assessments.
An assessment consists of a single substance and one or assessment items.
Review the input and correct where necessary
Select assessments for execution and
push the calculate button to start the simulations
View reports, graphs and maps

Figure 4. Major steps of a GeoPEARL assessment.

3. Use the assessment wizard to define an assessment.
4. Check the settings within the assessment and correct if necessary.
5. Perform the calculations by selecting the assessments and push the calculate button to start the calculations.
6. Review the results.

The five steps are elaborated in a little bit more detail below.

Step 1. Add or edit a substance.
To create a new substance, do the following:
- from the main screen, select View Substances from the drop down menu at the top to go to the Substances form;
- click + on the navigator to add the parent substance;
- the following properties must always be specified by the user:
  - in the General tab, specify a unique code, a name, the molar mass, the saturated vapor pressure and the solubility in water;
  - in the Freundlich sorption tab, specify the coefficient for sorption on organic matter;
  - in the Transformation tab, specify the substance half-life;
- if necessary, repeat the last two steps for the metabolites;
- if metabolites are involved, build the transformation scheme;
- Click Close when all done to return to the main screen.

More information on editing substance properties can be found in section 2.6.

Step 2. Add or edit one or more application scheme(s)
To create a new application scheme, do the following:
- from the main screen, select View Application Schemes from the drop down menu at the top to go to the Application Schemes form;
- click + on the navigator of the Application Schemes box (left-hand side of form) to add an application scheme;
- fill in a unique code and a name;
- click + on the navigator of the Applications box to add an application;
- Select the type of application and fill-in the other application parameters;
- repeat the last two steps if a substance is applied multiple times a year;
- Click close when all done to return to the main scheme.

More information on editing application schemes can be found in section 2.7.

Absolute applications only
Unlike in FOCUS PEARL 2.2.2, in GeoPEARL it is not possible to specify pesticide applications relative to crop emergence (so-called relative applications). The reason is that in GeoPEARL the crop emergence dates are part of a fixed spatial schematization, which cannot be manipulated by the user.

Step 3. Run the wizard
Press the Wizard button on the main screen to start a GeoPEARL assessment.

- Specify a name, the spatial detail wanted (i.e. the number of plots) and the substance for which GeoPEARL should be run. In order to get a reliable estimate of the 90th percentile of the leaching concentration, the number of plots should be at least 250. When done, select Next;
- Select a crop, an application scheme and the application interval. Then select Add.
- Repeat the last step for all combinations of crops and application schemes to be included in the assessment;
- Select Finish to go back to the main form.

Step 4. Refinement
GeoPEARL has now created an assessment. This assessment has already been selected for execution. Before actually running the model, it is advisable to review the most important model inputs. Where necessary, changes can be made.

Step 5. Running GeoPEARL
Press the Calculate button on the main screen to actually run the model. The actual run-time for the model is hard to predict, as it depends on the hardware, the number of assessment items and the number of plots that you have included. Anyhow, a typical GeoPEARL assessment will take at least five hours. We therefore recommend to use state-of-the-art hardware only. When an assessment is ready, you will see the 'Results' column changing to Yes. If something has gone wrong, the Error button will become active.

Step 6. Review results
- Press the Report button to review the summary report. This report contains, amongst others, the 90th percentile of the leaching concentration at the area of use, which is the target variable in the Dutch registration procedure;
- Press the Graphs and Maps button to view maps of the leaching concentration, maps of terms of the substances balances, etcetera.

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2.4 The projects form

The project form can be accessed from the main screen (see section 2.5). The projects form allows you to organize your data. Existing projects can be selected in the browse box (upper part of form). The navigator allows you to create or delete projects. An appropriate description can be added in the edit part.

2.5 The main screen

This form (figure 5) is the central point from where you can access the different tables of the database, run the wizard and review model inputs and model outputs. Most of the steps described in section 2.3 will be carried out from the main screen. You can use buttons, the main menu or shortcut keys to navigate through the GeoPEARL User Interface.

The main menu
The main menu can be used for easy access to various parts of the GeoPEARL user interface:

- Use File submenu to open another database (Key combination: Alt-F-O) or to exit GeoPEARL (Alt-F-X);
- Use the View submenu to directly jump to the projects form (Alt-V-P), the substances form (Alt-V-S) or the applications form (Alt-V-A);
- Use the Calculate submenu to start the calculations (Alt-C-C) or to select/unselect all assessments for execution;
- Use the Assessment submenu to run the Wizard (Alt-A-W), to move an assessment to another project (Alt-A-M) or to archive an assessment (Alt-A-A);
- Use the Help submenu to activate the help function.

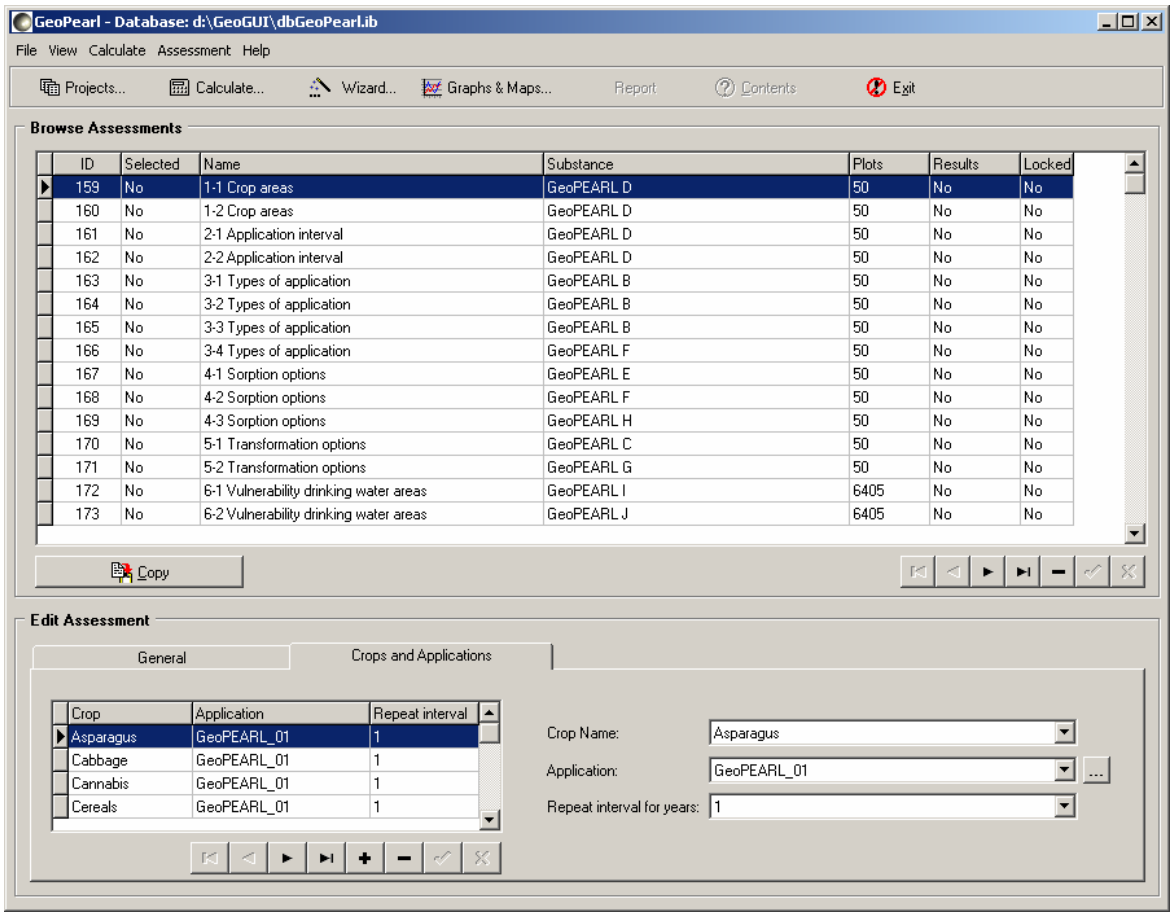

GeoPearl - Database: d:\GeoGUI\dbGeoPearl.ib
File View Calculate Assessment Help
Projects... Calculate... Wizard... Graphs & Maps... Report Contents Exit
Browse Assessments
ID Selected Name Substance Plots Results Locked
159 No 1-1 Crop areas GeoPEARL D 50 No No
160 No 1-2 Crop areas GeoPEARL D 50 No No
161 No 2-1 Application interval GeoPEARL D 50 No No
162 No 2-2 Application interval GeoPEARL D 50 No No
163 No 3-1 Types of application GeoPEARL B 50 No No
164 No 3-2 Types of application GeoPEARL B 50 No No
165 No 3-3 Types of application GeoPEARL B 50 No No
166 No 3-4 Types of application GeoPEARL F 50 No No
167 No 4-1 Sorption options GeoPEARL E 50 No No
168 No 4-2 Sorption options GeoPEARL F 50 No No
169 No 4-3 Sorption options GeoPEARL H 50 No No
170 No 5-1 Transformation options GeoPEARL C 50 No No
171 No 5-2 Transformation options GeoPEARL G 50 No No
172 No 6-1 Vulnerability drinking water areas GeoPEARL I 6405 No No
173 No 6-2 Vulnerability drinking water areas GeoPEARL J 6405 No No
Copy
Edit Assessment
General
Crops and Applications
Crop Application Repeat interval
Asparagus GeoPEARL_01 1
Cabbage GeoPEARL_01 1
Cannabis GeoPEARL_01 1
Cereals GeoPEARL_01 1
Crop Name: Asparagus
Application: GeoPEARL_01
Repeat interval for years: 1

Figure 5. The main form of the GeoPEARL User Interface.

The lower part of the screen gives information on browsed assessments. Furthermore you can indicate here the amount of information that will be shown on the screen during the calculation. When you check ‘detailed screen output’ more information will be shown on the screen during the calculations. This will, however, slow down the simulations.

2.6 Editing substances

The substances form is accessible from the main form of GeoPEARL. GeoPEARL can simulate the fate of a parent pesticide and its formation products (metabolites) in soil. This implies that both the properties of the individual compounds, and the transformation scheme have to

be parameterized. Both are accessible from the pesticides form. Input must be carried out in the following order:

- definition of the properties of the individual compounds;
- definition of the transformation scheme. This step can be ignored if only one compound is simulated.

At least one compound, the parent compound, must be introduced. This compound will be applied, deposited, etcetera. The user can make a compound a parent compound by checking the 'parent' check box in the general tab of the substances screen (see next section).

2.6.1 Editing individual compounds

The substances form consists of five tabs. These tabs are described below.

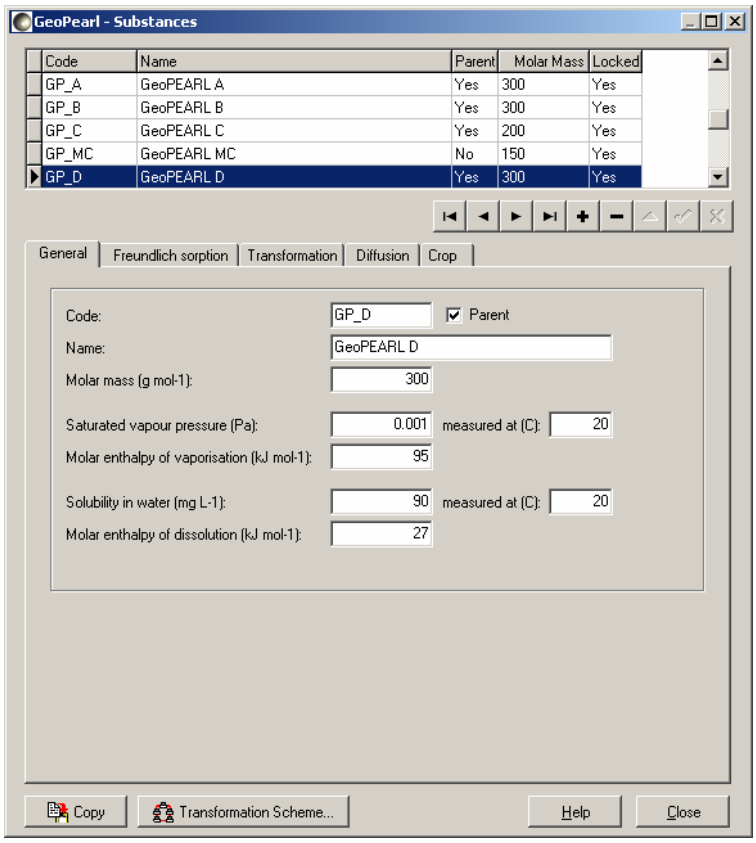


Figure 6.The substances form

General tab

In this tab, the user enters the general compound properties. A *unique* code and the compound name must be introduced into the code and name fields. The maximum length of the code is five alphanumerical characters. The following parameter to be introduced is the molar mass. Data on molecular masses of compounds are reported in Tomlin (1994). GEOPEARL then needs the saturated vapor pressure (PreVapRef), the temperature at which this parameter is determined (TemRefVap), the molar enthalpy of vaporization MolEntVap, the solubility of pesticide (SlbWatRef), the temperature at which the water solubility is obtained (TemRefSlb) and the molar enthalpy of dissolution (MolEntSlb). These properties can be taken from a

handbook on chemical properties of pesticides (e.g. Tomlin, 1994, Hornsby *et al.*, 1996). See section 3.2.8 of the FOCUS PEARL manual for further guidance.

Freundlich sorption tab

The sorption of compounds is described with a Freundlich equation (eqn. 41). See section 3.2.6 of the FOCUS PEARL manual for guidance and backgrounds. The Freundlich tab consists of three parts:

– the first part contains parameters describing the Freundlich coefficient;
– the second part contains the reference concentration and the Freundlich exponent;
– the third part deals with non-equilibrium sorption.

In the first part of the Freundlich tab, the user must make a choice between one of the three options that GeoPEARL has available to calculate the Freundlich coefficient (OptCofFre). The most common approach (OptCofFre is 'Kom, pH-independent') is to calculate the Freundlich coefficient from the organic matter content and the coefficient for sorption on organic matter (eqn. 42). If OptCofFre is set to 'Kom, pH-dependent', the Freundlich coefficient is calculated with eqn. 43. This equation applies to the sorption of weak-acids. In some cases the sorption of pesticides is dependent on other soil properties than the organic matter content (e.g. oxide content or clay content). Therefore, an option is included in GeoPEARL to relate the sorption to other soil characteristics than organic matter ('KF, dependent on soil components').

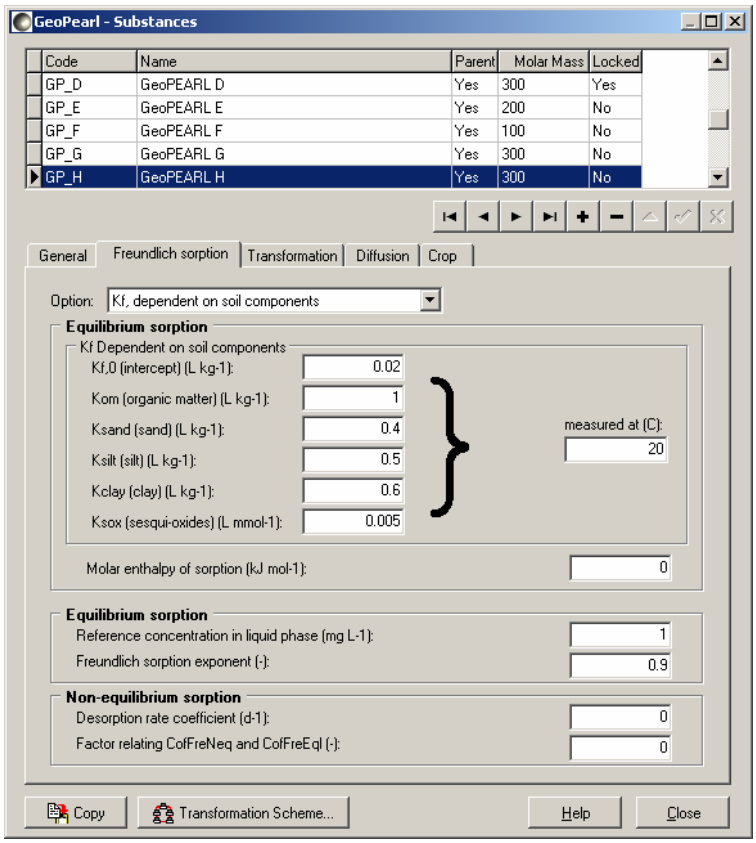


Figure 7. The Freundlich tab of the substances menu

For the moment this option is restricted to parameters that are available in the soil database distributed with GeoPEARL (i.e. soil texture, soil organic matter and sesqui-oxide content). The Freundlich coefficient is now calculated with eqn. 45.

If OptCofFre is set to 'Kom, pH-independent', only one additional parameter has to be introduced, i.e. the coefficient for sorption on organic matter, $K_{om,eq}$ (KomEql).

If OptCofFre is set to 'Kom, pH-dependent', two coefficients for sorption on organic matter must be specified (section 3.2.8 of FOCUS PEARL manual), i.e. KomEqlAcid ($K_{om,eq,ac}$) and KomEqlBase ($K_{om,eq,ba}$). In addition, the negative logarithm of the dissociation constant (pKa) and a pHCorrection are required.

If OptCofFre is set to 'Kom, soil dependent', you can relate the Freundlich sorption coefficient to one or more soil components, i.e. organic matter, sand, silt and sesqui-oxides. The overall sorption coefficient is a linear combination of the contributions of the components (eqn. 45). For each soil component, you must specify a sorption coefficient, i.e. KomEql for sorption on organic matter, KSandEql for sorption on sand, KSiltEql for sorption on silt, KClayEql for sorption on clay and KOxEql for sorption on sesquioxides. You also must specify the contribution not accounted for by any soil component (the constant of the linear regression equation, KFEql0). You must enter a value in each of the boxes; enter a value of zero if there is no contribution of that particular soil component. The K_{om} on this screen is stored at the same location in the database as the K_{om} possibly entered via the screen of the option K_{om}, pH-independent; that value will be overwritten.

The second part of the Freundlich tab contains two parameters. The reference concentration in the liquid phase (ConLiqRef) must be within the concentration range of the simulation study. Its default value is 1 mg L^{-1}. The Freundlich sorption exponent, n (ExpFre) is also required.

Non-equilibrium sorption is described with equation (47). This equation requires two additional parameters, i.e. the desorption rate coefficient, k_d, and the factor describing the ratio $K_{F,ne}/K_{F,eq}$, where $K_{F,ne}$ is the Freundlich coefficient at the non-equilibrium site and $K_{Fe,eq}$ is the Freundlich coefficient at the equilibrium site (FacSorNeqEql).

The desorption rate coefficient should be specified in the CofRatDes record. Please notice that non-equilibrium sorption will not be simulated if CofRatDes is set equal to zero. See further section 3.2.7 of FOCUS PEARL manual.

The transformation tab

In this tab, the user has to specify parameters that affect the transformation rate of the compound. The transformation half-life time must be input in the half-life field (DT50Ref). This half-life should refer to the half-life in the top soil (plough layer) under optimal moisture conditions (pF = 2). The temperature reflecting the experimental conditions during the incubation study (TemRefTra) must also explicitly be introduced.

An important difference with the transformation form in FOCUS PEARL is the presence of a half-life option field (OptDT50). This field can have two values, i.e. 'input' and 'calculate'. If set to 'input' GeoPEARL uses one DT_{50} value for the entire country. This value is equal to the value introduced in the half-life field. When choosing 'Calculate', pedotransfer functions are applied to relate the transformation half-life to soil components (see eqn. 62). The result is a spatially distributed half-life value. When choosing this value, you need to specify the parameters of the pedotransfer function.

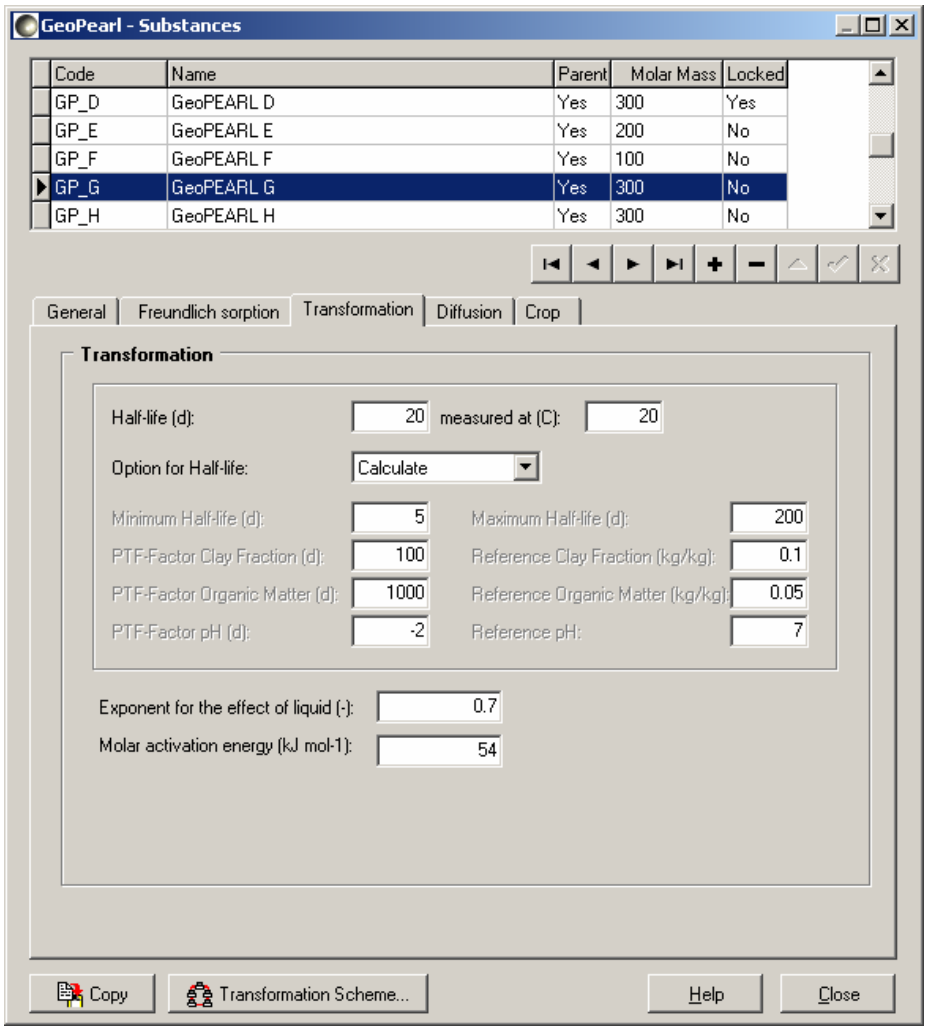


Figure 8. Input screen for soil dependent transformation parameters.

The pedotransfer function for transformation contains parameters for the dependence on the clay fraction (FacDT50Clay), the organic matter fraction (FacDT50Om) and the pH of the soil (FacDT50pH). The overall DT_{50}, under reference conditions, is taken to be a linear combination of the three components. Notice that the factors in the pedotransfer function have a unit, namely day. All fields must be filled, enter zero when the transformation is independent of a particular soil component. The user must also specify reference conditions for each of the three components (see eqn. 62), i.e. FraClayDT50Ref, CntOmDT50Ref and pHDT50Ref. Be careful that the reference conditions are entered as *fractions* for clay and organic matter content, not as percentages. Finally, you may specify the minimum (DT50Min) and the maximum

values (DT50Max) for the half-life; the model will use these values if the results of the calculations are beyond the range of these limits. In this way you can prevent GeoPEARL from extrapolating outside the range for which the pedotransfer function is valid.

In the lower part of the tab, the user must specify whether the incubation experiment has been carried out under optimum moisture conditions (OptCntLiqTra). As shown in eqn. 61, optimum moisture conditions are conditions wetter than field capacity (i.e. wetter than *p*F 2). If the incubation experiments have been carried out at moisture contents dryer than field capacity (i.e. dryer than *p*F 2), the optimum conditions checkbox must *not* be marked, and the user must additionally specify the moisture content during incubation (CntLiqTraRef). The temperature dependence of transformation is described with eqn. 60; the molar activation energy must be given (MolEntTra). The effect of soil water on the rate coefficient is described with eqn. 61, this equation requires an exponent (ExpLiqTra). See section 3.2.9 of FOCUS PEARL manual for further information on transformation parameters.

Example input for a substance with a spatially distributed half-life

Suppose you have a substance for which the transformation is dependent on soil organic matter, with a half-life (pF = 2, top soil, 20 °C) of 60 days in a soil with an organic matter fraction of 0.05 and a regression coefficient of 500 days. Furthermore, the range of the organic matter fractions in the measurements is between 0.005 and 0.10, corresponding with a range of half-lives from 37.5 days to 85 days. Suppose you want to use this range to define a minimum and maximum half-life. In this case you enter:

- 60 days for the reference half-life, $DT_{50,r}$
- select calculate
- 37.5 days for the minimum half-life
- 85 days for the maximum half-life
- 500 days for the PTF-factor for organic matter, f_{om}
- 0.05 kg kg^{-1} for the reference organic matter, $m_{om,r}$
- 0 for the other PTF factors and reference conditions, f_l, $m_{l,r}$, f_{pH} *and* pH_r

In a soil containing with an organic matter content of 0.01, GeoPEARL will use a half-life of 40 days for the top soil at 20 °C and pF = 2, according to eqn. 62: (40 = 60 + 500 *(0.01 – 0.05)).

The diffusion tab

The diffusion coefficients of pesticides in pure water (CofDifWatRef) and air (CofDifAirRef) are compound properties and must be specified in the diffusion tab. Parameters for the relative diffusion coefficient are soil dependent and cannot be manipulated by the user. The diffusion coefficients are temperature dependent. The user can specify one reference temperature, which applies to both the diffusion coefficient in air and the diffusion coefficient in pure water (TemRefDif).

The crop tab

GeoPEARL has modules to simulate canopy processes and root uptake. Both modules have to be parameterized in this tab.

As the transformation scheme (Figure 31) applies to products formed in soil, the canopy processes module considers the parent compound only. Processes that occur at the plant canopy

are volatilization, penetration into the plant and (photochemical) transformation (page 67). These processes are described with first-order rate reactions. The user can make a choice between a lumped description of the processes at the crop canopy, or a full description of dissipation (canopy processes combo box; OptDspCrp). If set to 'Specified', the user must specify the half-life due to penetration (DT50PenCrp), volatilization (DT50VolCrp) and transformation (DT50TraCrp). If set to 'Lumped'. an overall half-life (DT50DspCrp) is sufficient. The wash-off of pesticides is described with a zero-order equation with one parameter (FacWasCrp).

The only parameter in the equation for uptake of pesticides (eqn. 63) is the coefficient for the uptake by plant roots, FacUpt. See further section 3.2.11 of FOCUS PEARL manual.

2.6.2 The transformation scheme form

After the user has defined the properties for all individual compounds (section 2.6.1) to be considered in the simulation, the transformation scheme (table FraPrtDau) can be build. The transformation scheme form can be accessed from the substances form, using the 'transformation scheme' button. Before proceeding, read section 3.2.1 of FOCUS PEARL manual for guidance on deriving transformation fractions and look at Figure 31 for an example of a transformation scheme.

Information about formation products and fractions must be entered *for each compound considered*. If, for example, the user has defined one parent product (PEST) and two metabolites (e.g. MET1 and MET2), the transformation scheme form must be entered three times, i.e. one time from the PEST form, one time from the MET1 form and one time from the MET2 form.

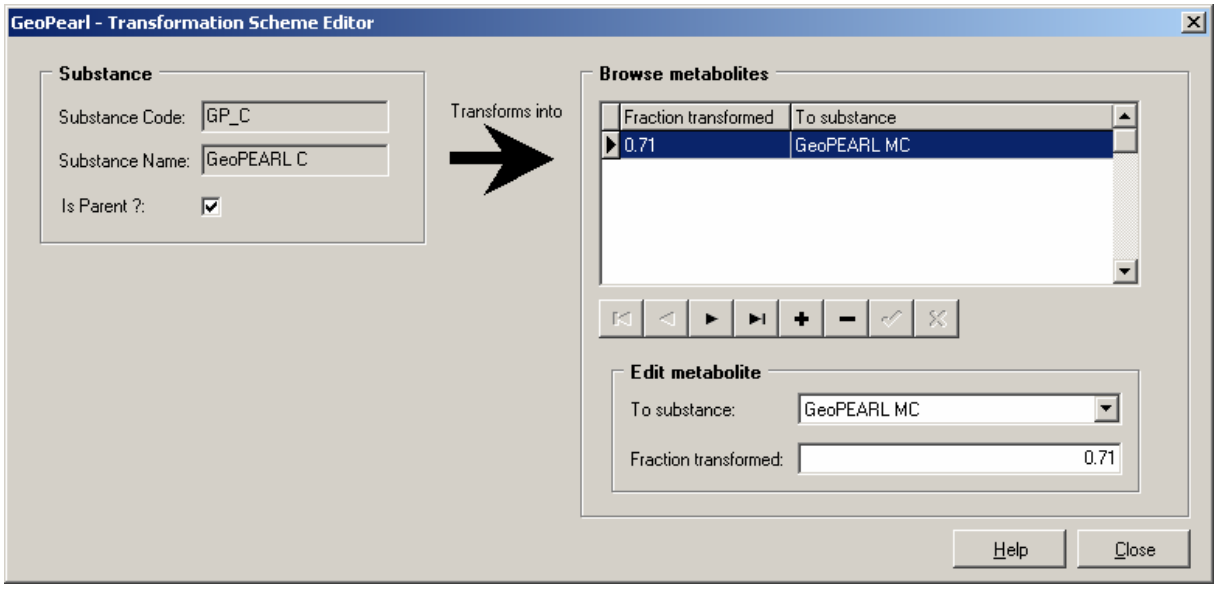


Figure 9. The transformation scheme form

Start with the definition of the transformation scheme of the parent (PEST). Go to the PEST form and press 'transformation scheme'. The left part of the form shows the parent product and some of its main properties. You cannot edit this part of the screen. To the right you will see the metabolites. By default, no metabolites are specified. If you leave these parameters

unchanged, PEARL will *not* simulate metabolites. Extra metabolites can be added using the + button in the browse toolbar. Pick a metabolite from the 'to substance' list. If you want to add more metabolites, repeat the preceding two steps. After you have selected all metabolites, enter the transformation fractions.
Repeat the steps in the last paragraph for the two other metabolites. To achieve this, first go to the MET1 and MET2 forms, then press 'transformation scheme'.

2.7 Editing application schemes

2.7.1 Application schemes

The application schemes form is accessible from the main menu of the main screen (View-Application Schemes). The entire events scheme can be repeated annually, biennially or triennially using the 'application interval' option at the main screen.

Event schemes (Events) can be added with the + button of the navigator. You can also copy an existing event scheme. Event schemes should be given a *unique* code for reference and a description. Use the 'Events' button to define the individual events.

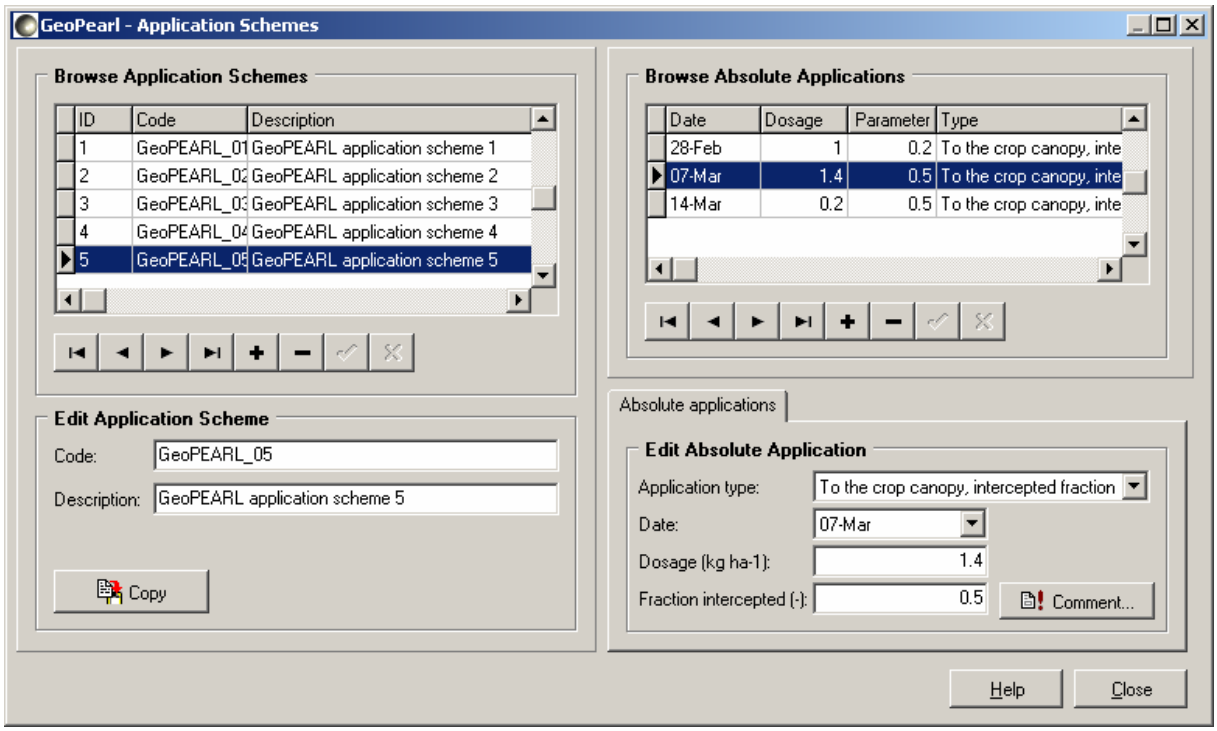


Figure 10. The application schemes form

2.7.2 Applications

Add a new event with the + button of the navigator or copy an existing event. In the lower half of the screen, the event has to be further defined. First define the application type: 'application to the soil surface' (AppSolSur), 'injection' (AppSolInj), 'incorporation' (AppSolTil) or 'application to the crop canopy, interception fraction supplied by the user' (AppCrpUsr). Then enter the date and the dosage. Normal date format can be used. The year is not required

as GeoPEARL always repeats the entire application scheme annually, biennially or triennially. In the case of injection or incorporation, you must additionally supply the incorporation or injection depth.

2.8 Composing an assessment with the Assessment Wizard

As described in section 2.1, an assessment is the basic entity of GeoPEARL. An assessment is carried out for a single substance and for one or more assessment items, which are combinations of crops and application schemes. Assessments are composed using the Wizard button on the main screen. You can compose an assessment after the substance and the application schemes that you want to use in your GeoPEARL calculations are defined. After selecting the assessment wizard, the following screen appears:

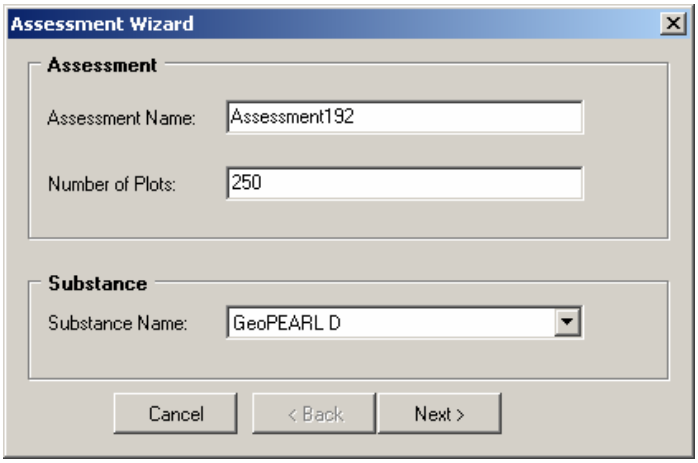


Figure 11. First screen of the assessment wizard.

Type the name of the assessment and define the number of plots to be included in the assessment. You can enter a number between 2 and 6405. However, for a reliable calculation of the 90th percentile of the leaching concentration, at least 250 plots should be used (see chapter 4); use a lower number only for test runs. If the given number of plots is larger than the number of plots available for a certain crop, then GeoPEARL calculates for the maximum number available.

Subsequently select a substance (defined earlier) and click the Next button. The screen shown in figure 12 will appear. Select a crop (see text box), an application scheme (defined earlier) and a repeat interval for the application scheme (i.e. annually, biennially or triennially) and click the Add button. Repeat this step for every crop you want to be included in the assessment. It is not possible to select a crop twice (with different application schemes) in a single assessment. Press the Finish button after having selected all combinations for the assessment. You return to the main screen, from where you can work further.

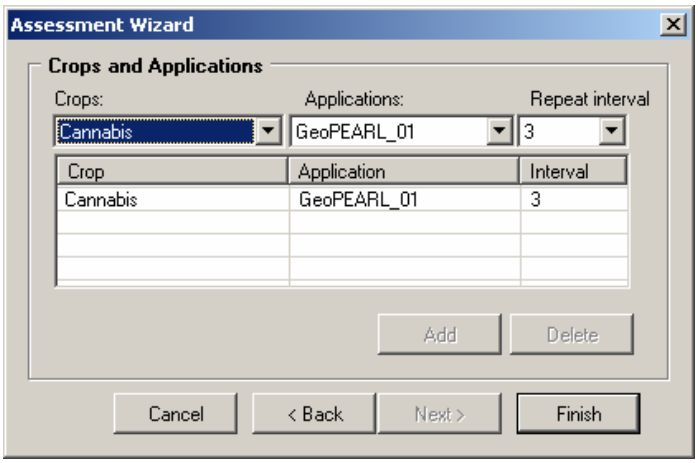


Figure 12. Second screen of the assessment wizard.

Crops
Crops are used in GeoPEARL to identify the area of use of a plant protection product. You can choose from 26 entries. Most of the entries consist of a single crop or a crop group and it will be quite clear from the name what is meant. For example, the entry 'potatoes' stands for all potato crops, so including seed potatoes, starch potatoes and potatoes for consumption. The following entries need explanation:

- Fallow: agricultural area, indicated not to be used for production of crops for some period;
- Plants for commercial purposes: caraway, flax, poppy seed and rapeseed;
- Remaining agricultural crops: crops not identified by other entries, usually these crops individually have an acreage up to a few hundred hectares;
- Total agricultural area: area of all crops (including fallow) together;
- Total non-urban area: total non-built-up area, i.e. agricultural area and nature area.

The 24 crops / crop groups (including fallow) can be combined in an assessment. For example, it is possible to select both sugar beets and potatoes in an assessment. It is, however, impossible to combine individual crops with the total agricultural area or the non-urban area; this would lead to overlap in areas. Likewise it is impossible to combine the agricultural area and the total area.

2.9 Checking assessment definitions

Back at the main screen you can check the definitions of the assessments. If necessary, you can make changes immediately by editing an assessment in the main screen. The main screen gives an overview of the most important items of the assessment, in two tabs. All the assessment items can be changed in the respective tabs.

2.10 Running the model

An assessment can be selected for execution by double clicking the respective assessment. Multiple assessments can be selected; all selected assessments are executed by pressing the 'Calculate' button on the main screen. In the main menu, you can select or deselect all assessments in a project at once (menu item Calculate).

After starting the calculations, a GeoPEARL progress screen will appear. This screen roughly indicates the progress of the execution at the bottom of the screen. On the right side of the progress bar you see a Suspend button (figure 13). This button can be used to temporarily stop the execution. This button is active only in the calculation phase; it is not active when GeoPEARL is preparing the input for the calculations and when GeoPEARL is preparing output. *Caution: the suspend button stops all PEARL and GeoPEARL calculations on a machine, not only the calculations that were started from the GeoPEARL window from which you started the calculations for this assessment.* A warning appears after pushing the button; you have to confirm that you want to suspend the calculations. You can resume the calculations by clicking 'Calculate' again; GeoPEARL will continue with the first unfinished plot.

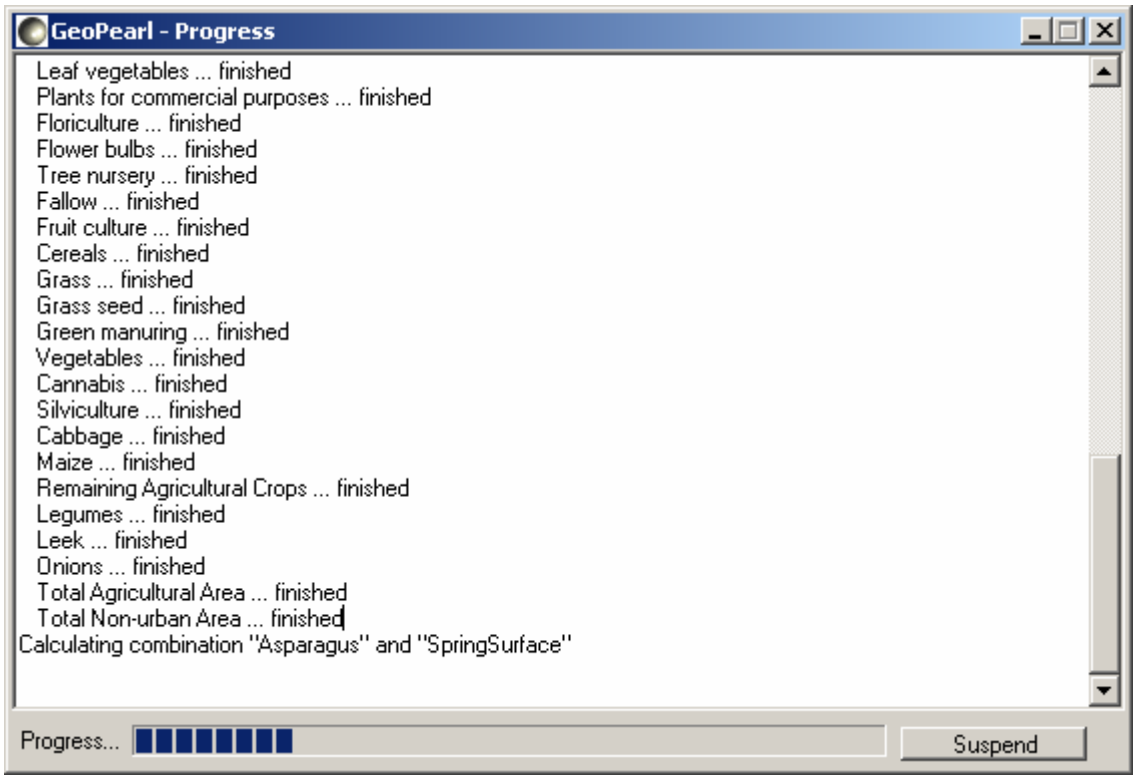


Figure 13. Screen indicating the progress of model execution.

2.11 Reports showing the target variable for registration

When GeoPEARL has terminated successfully, you will see that the Results column is set to Yes. Also, the Reports button will become highlighted. You can use this button to view a summary report, which shows the 90th percentile of the leaching concentration for the area of usage. As described in the text box in section 2.8, this area is represented by the total area of the crops selected when composing an assessment. See also section 2.5 of the GeoPEARL report for explanation of the area of usage. The reports contain information on the leaching concentration of all substances, including metabolites.

The target variable
The 90th percentile of the leaching concentration is calculated in a number of steps:
1. For each plot average leaching concentrations are calculated for 20 calculation periods. The length of the calculation periods is one year in the case of annual applications, two years in the case of biennial applications and three years in the case of triennial applications (conform FOCUS, 2000).
2. From these 20 values, the median value is taken. The result is considered the leaching concentration of a plot.
3. The 90th percentile in space is calculated using the median values of all plots.

Notice that in the Dutch registration procedure, the target variable is the median concentration in time and the 90th percentile in space. This is different from the FOCUS procedure, where the 80th percentile in time is combined with an approximate 80th percentile in space.

2.12 Viewing maps and graphs

By clicking the Graphs and Maps button, the user has fast access to all spatially distributed model inputs and model outputs. This option is extremely powerful when analyzing the behavior of the model behavior. Three major groups of variables can be accessed:
1. Spatially distributed model input parameters, which fall apart into two categories, i.e. soil parameters and crop areas. These parameters can be accessed through the 'Echo of Input' tab. As mentioned in section 2.8, crop areas are used as a proxy for the area of usage.
2. Output parameters that are available for the total area of use; i.e. for the area of all crops included in the assessment.
3. Output parameters that are available for assessment items, i.e. for specific combinations of crops and application schemes included in an assessment.

It is always possible to review the model inputs, the other two tabs are only visible if an assessment has run successfully.

Some of the maps are prepared automatically after finishing the calculations. It will take only a few moments to present these maps on the screen. Other maps are prepared only upon request of the user. The preparation of these maps, i.e. the selection of appropriate results, may take several minutes.

2.12.1 Viewing input parameters

Maps of input parameters and maps of crop areas are available in the 'Echo of Input' tab (figure 14). For viewing input parameters, check 'Map – Soil properties' and select the appropriate parameter from the drop-down box and the depth for which you want the parameter to be visualized. To view the crop areas, check 'Map – Crop area' and select the crop from the drop-down box.

2.12.2 Viewing output parameters for the total area of usage

If you want to graph results for the total area of usage, select the 'Area of usage' tab (figure 15). This tab is only visible if results are available. You can choose between two graphs:
– the first graph shows the cumulative frequency distribution of the median leaching concentration of each plot;

– the second graph shows the cumulative frequency distribution of the 20th, 50th and 80th percentiles of each plot. This graph is an extension of the first graph; it shows the variability of the leaching concentration due to variability in weather conditions.

Both graphs can be shown for all substances in an assessment; i.e. the parent and, if applicable, the metabolites.

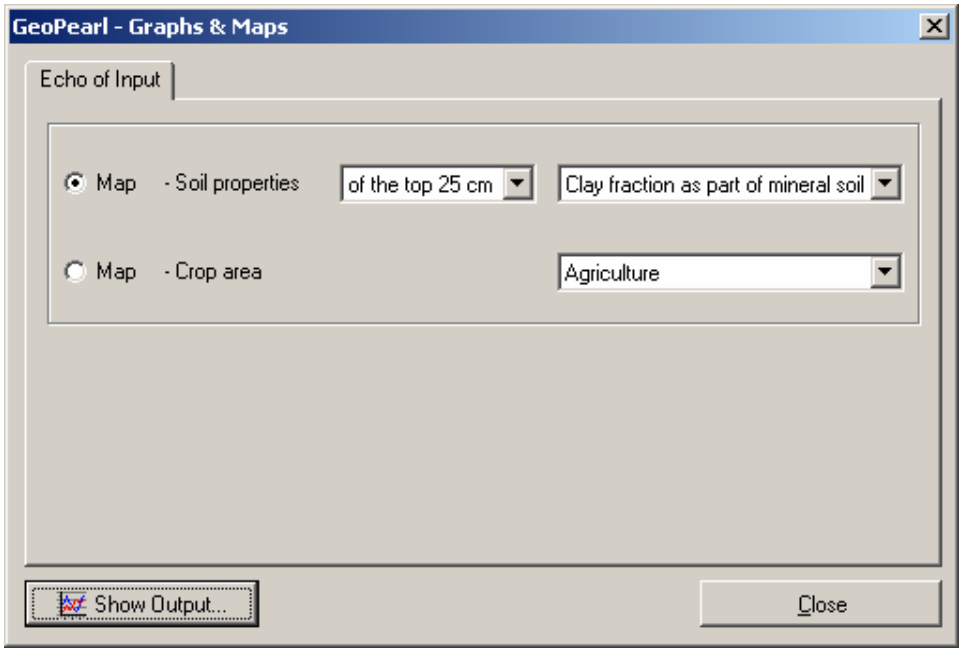


Figure 14. Screen for reviewing the input parameters

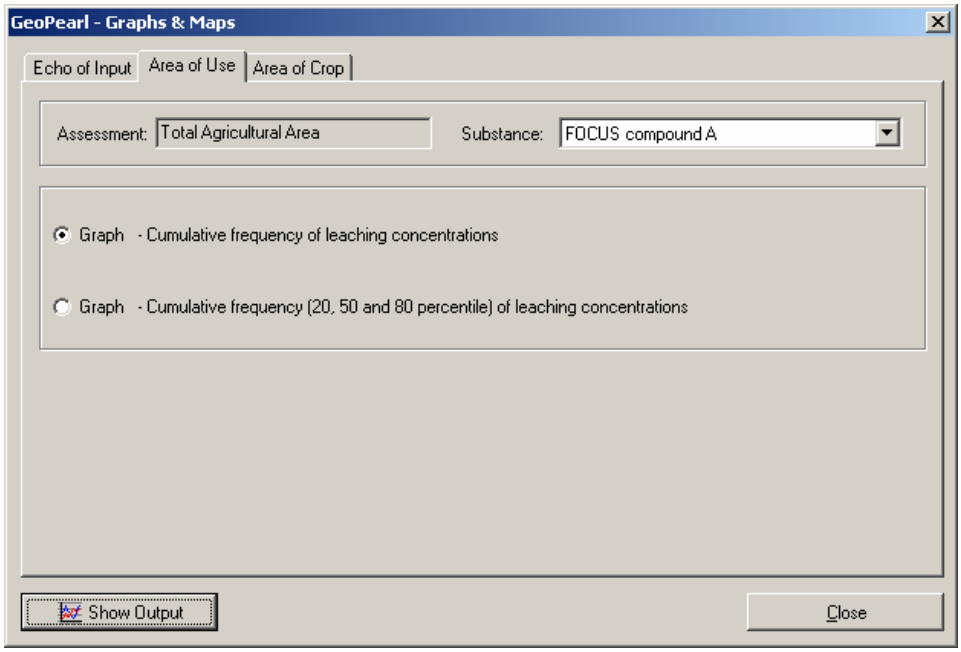


Figure 15. Screen for viewing output for the area of use of the substance in an assessment.

2.12.3 Viewing output parameters for individual crops within an assessment

If you want to graph results for the total area of usage, select the 'Area of crop' tab (figure 16). This tab is only visible if results are available. First select the substance for which you want to view the output You can choose between the following type of graphs:

- cumulative frequency distribution of the median leaching concentration. In contrast to the graph in previous section, this graph pertains to a single crop only;
- cumulative frequency distribution of the 20th, 50th and 80th percentile in time of the leaching concentration;
- maps of the leaching concentration;
- maps of terms of the water balance. A schematic overview of the water balance is presented in figure 20;
- maps of terms of the substance balance. A schematic overview of the substance balance is presented in figure 21.

All maps are presented with five classes, all classes have the same area (automatic legend scaling). In the case of the leaching concentration, it is also possible to create a map with preset classes. The advantage of a map with preset classes is that the trigger concentration of 0.1 µg L^{-1} is clearly visible.

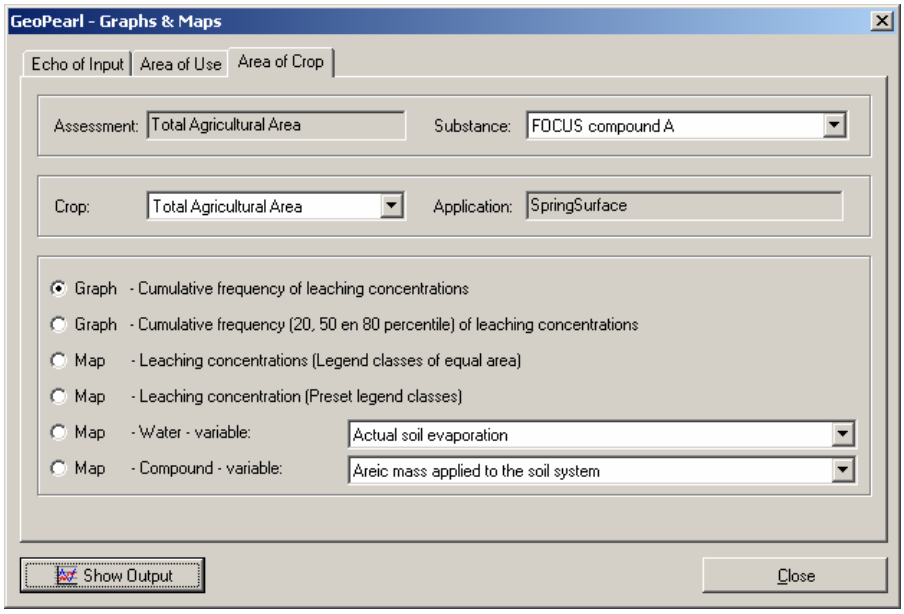


Figure 16. Screen for viewing output for individual crops within an assessment.

2.12.4 The viewer

GeoPEARL uses the graphical program XYWIN (Van Heerden and Tiktak, 1994) for all graphs and maps. Functions that are available within XYWIN are:

- Zooming: click the left mouse button to select a rectangle. *Warning: this function is only intended to analyze the map; it should not be used to 'read' the leaching concentration in your 'backyard'.*
- Statistics: you can use XYWIN to create frequency diagrams of maps. *Warning: if used for maps of the leaching concentration, this function may give different results than the*

cumulative frequency distribution generated by GeoPEARL itself. The reason is that blanks are threated in another way.
- Printing: Graphs can be printed by pressing CNTRL-P or by selecting print from the file menu.
- Export of graphics files: Use the File menu select Output. You can specify different output formats, like jpg, png, tiff and emf. If you want to incorporate a graph in a word processor like Word, we advise to use png format.

2.13 Archiving your assessment

The GeoPEARL User Interface has the possibility to export the information that is required to run the assessment to ASCII files. The structure of these files is described in chapter 3. This functionality can be accessed by selected Archive from the Assessment submenu at the main screen (or press Alt-A-A). The obtained files can be used:
- to archive your run;
- as input for the stand-alone version of GeoPEARL.

Please notice that it is currently not possible to import the obtained files into another GeoPEARL database. You must also archive the GeoPEARL database.

2.14 Directory structure for the GeoPEARL User Interface

The communication between the GeoPEARL User Interface and the GeoPEARL executables is through ASCII files. These files can also be used in combination with the stand-alone version of GeoPEARL, as described in chapter 3. Figure 17 shows the directory structure used by the GeoPEARL User Interface:
- The GeoPEARL root directory is the directory that you have specified during the installation
- The bin directory contains all executables
- The database directory contains the GeoPEARL database. The default name of the database is DbGeoPearl.ib.
- All ASCII files required by the GeoPEARL executable are stored in the DBGeoPEARL directory. *The actual name of this directory depends on the name of the database.* If, for example, the name of the database is bentazone.ib, the name of this directory would also have the name ‘bentazone’. The number of data directories is equal to the number of GeoPEARL databases.
- The next level is the Assessment directory. For each assessment that has been carried out with GeoPEARL, a directory is created. Directories are given numbers; the numbers correspond with the assessment number.
- Parallel to the Assessment directory, you will find the Schematisation directory. This directory contains all the ASCII files of the spatial schematisation (represented by an orange color in figure 18) and the output control file (ctr file).
- The Temp directory contains temporary files generated by the GeoPEARL executable.
- Within the assessment directory, you will find one or more assessment item directories. In this directory, you will find back the geo, cmp and app files (see section 3.2 for explanation).

– The output of an assessment item is written to the output subdirectory (the files with a blue color in figure 18).

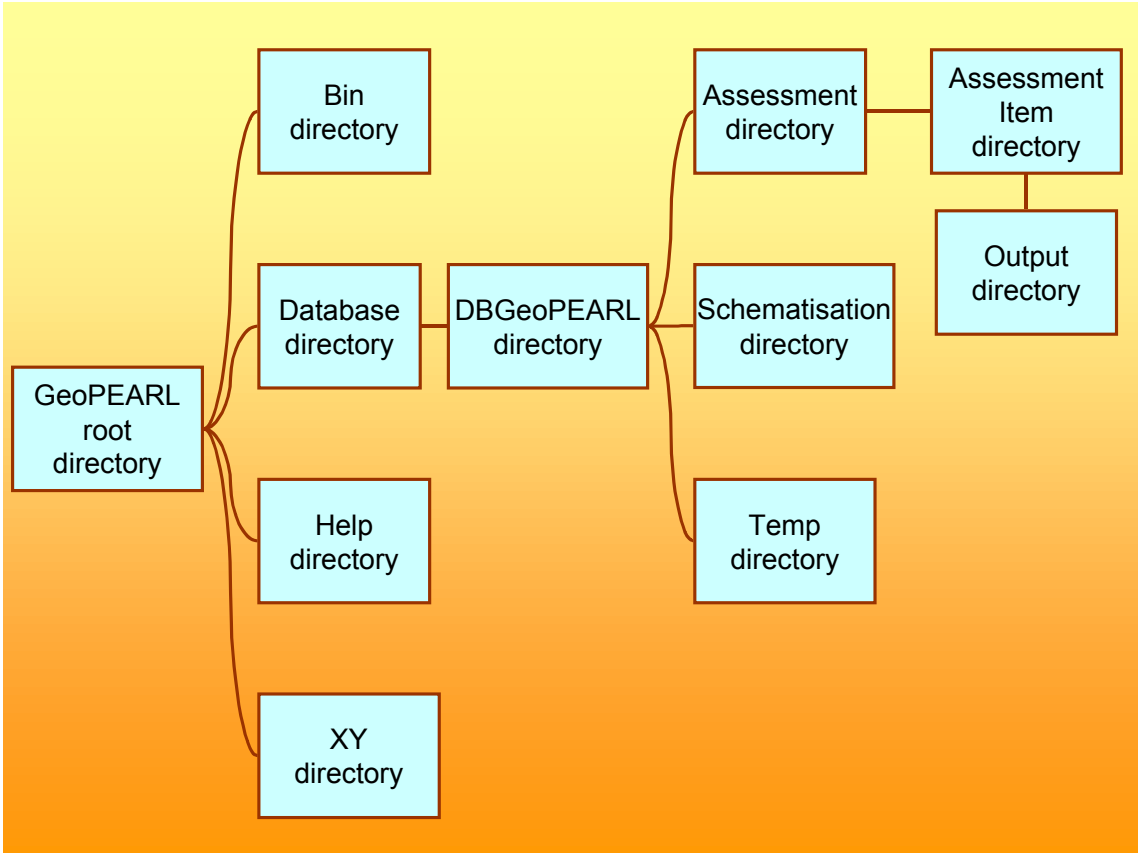


Figure 17. Directory structure for the GeoPEARL User Interface

2.15 Using another database

You can use multiple database with GeoPEARL. To do so, follow this procedure:

– goto the database directory and copy the database (i.e. the file with extension .ib). The name of this database should be different from the name of the original database;
– From the main menu, select File – and then 'Open GeoPEARL database' to open another database;
– GeoPEARL will now open the other database;
– When starting GeoPEARL, it will open the database that was in use when shutting down.

3 User's guide of the command-line version of GeoPEARL

This section describes the command-line version. It is described how the model can be applied to applications in which the user primarily wants to change the substance properties and the application schedule. You will see that the steps for running the stand-alone version of GeoPEARL are almost the same as the steps to be followed when using the GeoPEARL User Interface. This manual is dedicated to the Dutch application. If you want to use GeoPEARL for other countries, you first have to create a new spatial schematisation. Once done, the steps are exactly the same as in the Dutch application.

3.1 Performing an assessment with the stand-alone version

1 Install GeoPEARL according to the instructions in section 2.2.

2 Download the 'geopearl_1_1_1_ascii.exe' self-extracting archive from the PEARL website to get the input files for the stand-alone version of GeoPEARL. Put the files preferably into a directory *without spaces*.

3 Copy the contents of the Example directory to a new directory. Assign a unique directory to each assessment. You can, alternatively, copy assessments from the GeoPEARL User Interface (see section 2.14 for directory structure). Files generated by the GUI do, however, not have comment lines and are more difficult to understand.

4 Add a new substance to the compounds file and edit the substance properties (page 41).

5 Add a new application schedule to the applications file and edit it (page 44).

6 Edit the geo file.
   a Specify the directory structure (page 46).
   b Specify the control options of GeoPEARL (page 46).
   c Specify the required spatial resolution and the crop for which a registration is requested (i.e. plot selection; page 47).
   d Specify the substance and application schedule (page 49).
   e Request additional (detailed) output (optional, page 50).

7 Run the model (page 50).

8 GeoPEARL creates a number of output files, containing the substance and water balances and percentiles of the leaching concentration (page 51).

9 Use the 'percentiles.exe' executable to calculate the 90^{th} percentile of the leaching concentration and generate maps.

10 The tables can be imported in EXCEL for additional calculation or in a Geographic Information System to generate maps and regional-scale substance and water balances (page 57).

3.2 File structure

Figure 18 gives an overview of all files types. Each file type has its own extension, the extension may not be changed. There are three groups of files:

- Files that need to be edited in standard applications. These files are given a green color in figure 18 and are stored in the example directory.
- Files that contain the spatially distributed parameters. These files should not be changed, unless a new spatial schematisation is set-up by the user. These files are given an orange color in figure 18 and stored in the schematisation directory.
- Output files (blue color), which are stored in the output directory.

The position of all files can be changed (see further page 46). This report describes the green and blue files only, as these are the files that are relevant for standard applications. A description of the other files can be found at the PEARL website (http://www.pearl.alterra.nl).

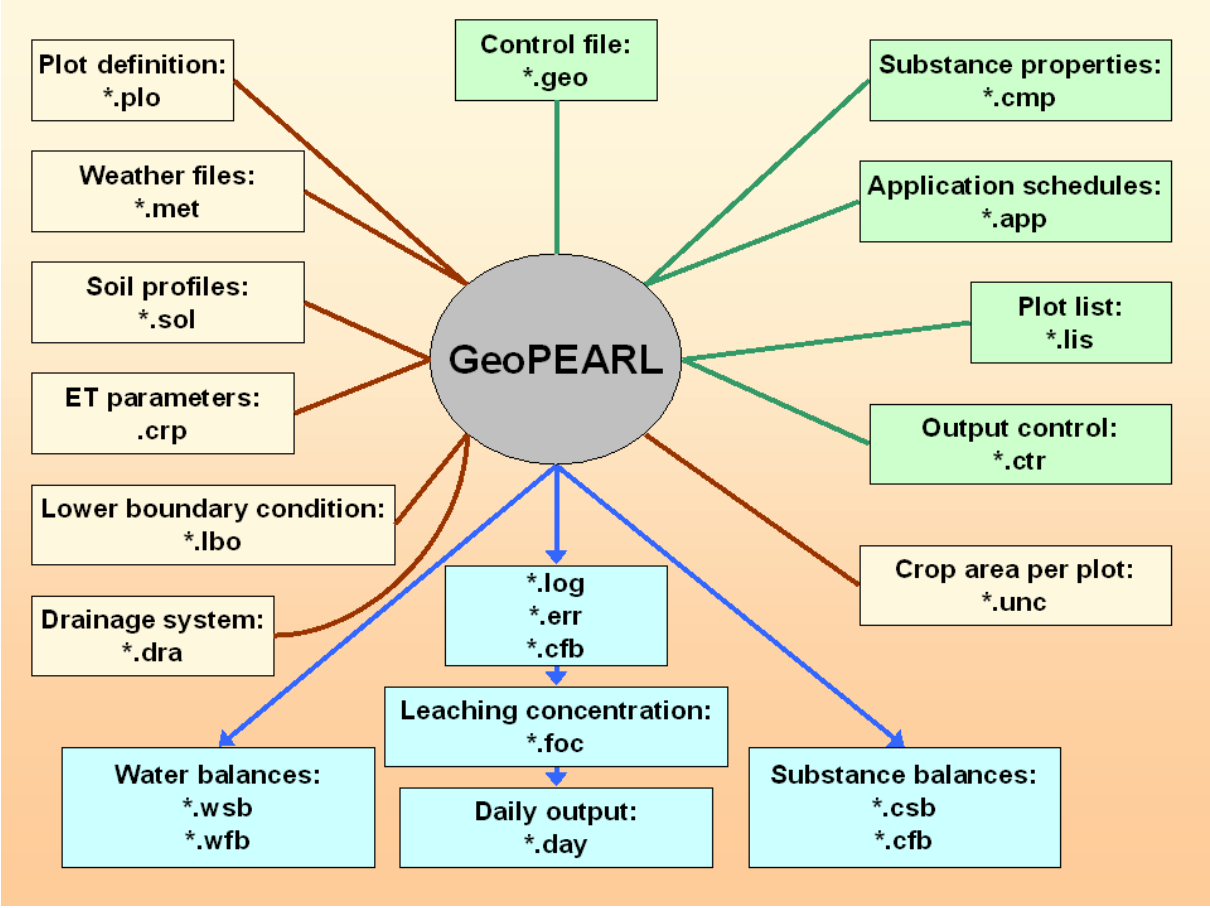


Figure 18. File structure of GeoPEARL. Files with a green color are stored in the assessment directory, files with an orange color in the schematisation directory. Only files with a green color need editing.

3.3 Creating an assessment with multiple assessment items

As described in section 2.1, a GeoPEARL assessment is carried out for a single substance, but may consist of several so-called *assessment items*. Assessment items are combinations of a crop for which a registration is asked and an application scheme. This implies that different

crops can have different application schemes. To carry out an assessment with more items, do the following:

1) After having created the geo file for the first crop, copy this file as many times as there are items in your assessment. If, for example, you have to do an assessment for maize, potatoes and cereals, create a file maize.geo, potatoes.geo and cereals.geo
2) In each geo file, assign the appropriate crop in the Crops table and the appropriate application schedule in the applications table. *Warning: these two variables are the only variables that can be different within an assessment! You can only use one substance within an assessment.*
3) Run the model for all items.
4) Use the percentiles.exe program to:
   a) calculate the overall 90th percentile of the leaching concentrations at the total area of usage;
   b) calculate the 90th percentile of the leaching concentrations for each assessment item individually;
   c) generate maps.

   The percentiles program should be run one time in an assessment.

The entire procedure is described in figure 19.

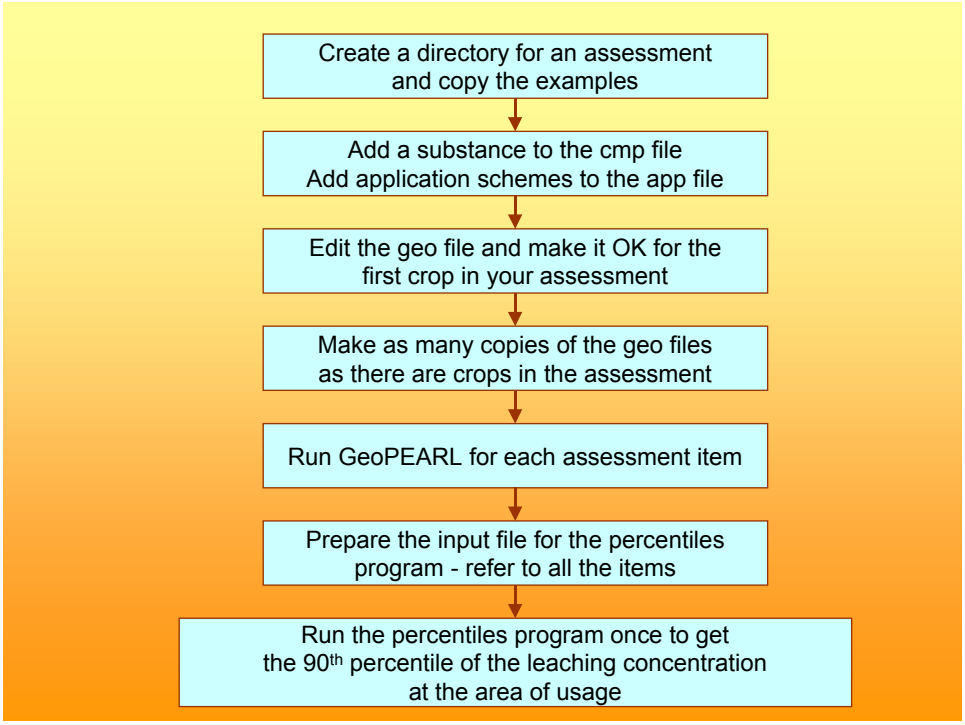

Create a directory for an assessment and copy the examples
Add a substance to the cmp file Add application schemes to the app file
Edit the geo file and make it OK for the first crop in your assessment
Make as many copies of the geo files as there are crops in the assessment
Run GeoPEARL for each assessment item
Prepare the input file for the percentiles program - refer to all the items
Run the percentiles program once to get the 90th percentile of the leaching concentration at the area of usage

Figure 19. Performing an assessment with multiple assessment items with the stand-alone version of GeoPEARL.

3.4 Adding and editing substances

Substance properties must be specified in the file with extension **cmp** (step 4 of 'Getting Started'). The substances file contains exactly the same information as the 'compound properties' section of the PEARL input file as described in section 4.2.9. of the FOCUS PEARL

user manual. For detailed information on substance properties, the reader is referred to this manual.

The substances file consists of two sections:

- A section containing generic substance properties. This section contains default parameters. These defaults can be overwritten by including them in the second, substance specific, section.
- A section with substance specific properties.

Below follows a listing of the generic part of the substances file. Please note that *the substance properties in this section do not have substance extensions*.

```
*-------------------------------------------------------------------------------
* Default substance parameters
* Parameters can be overwritten by including them into the compound section
* of the relevant pesticide

*-------------------------------------------------------------------------------
* Gas/liquid partitioning parameters
20.0              TemRefVap  (C)          .. measured at [0|40]
95.0              MolEntVap  (kJ.mol-1)   Molar enthalpy of vaporization [-200|200]
20.0              TemRefSlb  (C)          .. measured at [0|40]
27.0              MolEntSlb  (kJ.mol-1)   Molar enthalpy of dissolution [-200|200]
0.0               MolEntSor  (kJ.mol-1)   Molar enthalpy of sorption [-100|100]
20.0              TemRefSor  (C)          .. measured at [0|40]

*-------------------------------------------------------------------------------
* Uptake parameters
0.5               FacUpt     (-)          Coefficient for uptake by plant [0|10]

*-------------------------------------------------------------------------------
* Diffusion of solute in liquid and gas phases
4.3d-5            CofDifWatRef (m2.d-1)   Diff. coeff. in water [10e-5|3e-4]
0.43              CofDifAirRef (m2.d-1)   Diff. coeff. in air [0.1|3]
20.0              TemRefDif  (C)          ... measured at [10|30]

*-------------------------------------------------------------------------------
* Transformation rate parameters
20.0          TemRefTra (C)          Temperature at which DT50 is measured [5|30]
0.70          ExpLiqTra (-)          Exponent for the effect of liquid [0|5]
OptimumConditions OptCntLiqTraRef    OptimumConditions or NonOptimumConditions
1.0           CntLiqTraRef (kg.kg-1) Liq. content at which DT50 is measured [0|1]
54.0          MolEntTra (kJ.mol-1)   Molar activation energy [0|200]

*-------------------------------------------------------------------------------
* Sorption parameters
0.9               ExpFre     (-)          Freundlich sorption exponent [0.1|1.3]
1.0               ConLiqRef  (mg.L-1)     Reference conc. in liquid phase [0.1|-]
0.0               pHCorrection    (-)     pH correction [-2|1]

*-------------------------------------------------------------------------------
* Non-equilibrium sorption
0.00              CofDesRat  (d-1)        Desorption rate coefficient [0|0.5]
0.5               FacSorNeqEql (-)        CofFreNeq/CofFreEql [0|-]
```

For each substance to be simulated, the user must specify a substance specific section. Each of these sections starts with [substance_name] and ends with [end_substance_name], where substance_name should be replaced with the actual name of the substance. Parameters in the

specific sections overrule parameters in the default section. The following parameters must always be specified, as default values are not given:

- Table FraPrtDau: Specifies the parent-daughter relationships. See page 66 of FOCUS PEARL manual. If left empty, the model assumes that there are no relevant daughter products.
- OptCofFre: Method to describe the Freundlich sorption coefficient (page 66 of FOCUS PEARL manual). The Freundlich sorption coefficient can be specified pH-dependent or pH-independent. If OptCofFre is set to pH-independent, KomEql must be specified; if set to pH-dependent, KomEqlAcid, KomEqlBase and pKa must be given. The Freundlich sorption coefficient can also be made dependent on other soil parameters (option GeoPEARL). In this case the variables KFEql0, KomEql, KSandEql, KSiltEql, KClayEql, and KOxEql must be specified additionally.
- OptDT50: Method to describe the half-life of transformation. Can be set to Input or Calculate. In the first case, the reference half-life that is specified by the user applies to all plots included in the simulations. In the second case pedotransfer functions are applied to calculate soil dependent half-life values. If this option is chosen, additional parameters need to be specified (see page 44).
- DT50Ref: Half-life under reference conditions.
- KomEql: The sorption coefficient on organic matter. If OptCofFre is set to pH-dependent, two K_{om} values must be specified, i.e. one for acidic conditions (KomEqlAcid) and one for basic conditions (KomEqlBase). In addition, the negative logarithm of the dissociation constant (pKa) is required. For further details, read the FOCUS PEARL manual.
- PreVapRef: The saturated vapour pressure at reference temperature. Notice that the default reference temperature in GeoPEARL is 20 ^{o}C; if another temperature is needed, specify this temperature in the substance specific section.
- SlbWatRef: The solubility in water at reference temperature. The default reference temperature in GeoPEARL is 20 ^{o}C; if another temperature is needed, specify this temperature in the substance specific section.
- DT50DspCrp: The dissipation half-life at the crop canopy. This variable will ignored in the case of those pesticides that are applied directly to the soil.
- FacWasCrp: The wash-off factor from the crop canopy. This variable will ignored in the case of those pesticides that are applied directly to the soil.

```
*-------------------------------------------------------------------------------
* Substance specific substance properties. Parameters in this section must have
* a substance extension.
*
*-------------------------------------------------------------------------------

*-----------------------------------------------------------------------------------------
* CMPC = FOCUS compound_C

[CMPC]

table FraPrtDau (mol.mol-1)
0.71 C -> MET-C
end_table

pH-independent    OptCofFre_C                [pH-dependent|pH-independent|GeoPEARL]
Input             OptDT50_C                 Option for DT50 [Input|Calculate]
```

```
200.0             MolMas_C        (g.mol-1)   Molar mass [10|10000]
20.0              DT50Ref_C       (d)         Half-life time [1|1e6]
100.0             KomEql_C        (L.kg-1)    Coef. eql. sorption on org. matter [0|1e9]
1.d-10            PreVapRef_C     (Pa)        Saturated vapour pressure [0|2e5]
50.0              SlbWatRef_C     (mg.L-1)    Solubility in water [1e-9|1e6]
1.d6              DT50DspCrp_C    (d)         Dissipation  half-life on canopy [1|1e6]
1.d-4             FacWasCrp_C     (m-1)       Wash-off factor [1e-6|0.1]

pH-independent    OptCofFre_MET-C             [pH-dependent|pH-independent|GeoPEARL]
Input             OptDT50_MET-C               Option for DT50 [Input|Calculate]
150.0             MolMas_MET-C    (g.mol-1)   Molar mass [10|10000]
100.0             DT50Ref_MET-C   (d)         Half-life time [1|1e6]
30.0              KomEql_MET-C    (L.kg-1)    Coef. eql. sorption on org. matter [0|1e9]
1.d-10            PreVapRef_MET-C (Pa)        Saturated vapour pressure [0|2e5]
50.0              SlbWatRef_MET-C (mg.L-1)    Solubility in water [1e-9|1e6]
1.d6              DT50DspCrp_MET-C (d)        Dissipation  half-life on canopy [1|1e6]
1.d-4             FacWasCrp_MET-C  (m-1)      Wash-off factor [1e-6|0.1]

[end_CMPC]
```

If the sorption coefficient is *p*H-dependent, the following parameters must be specified (example substance E):

```
500.0             KomEqlAcid_E    (L.kg-1)    Coef. for eql. sorption on om - acid [0|1e9]
25.0              KomEqlBase_E    (L.kg-1)    Coef. for eql. sorption on om - base [0|1e9]
4.5               pKa_E           (-)         Coef. for influence of pH on sorption [0|14]
```

If the sorption coefficient is made dependent on other soil parameters (OptCofFre=GeoPEARL), the following parameters must be included in the substance section (see page 26 for further explanation):

```
0.02              KFEql0_H        (L.kg-1)    Regression coefficient [0|1e9]
1.0               KomEql_H        (L.kg-1)    Coef. eql. sorption on org. matter [0|1e9]
0.4               KSandEql_H      (L.kg-1)    Coef. eql. sorption on sand [0|1e9]
0.5               KSiltEql_H      (L.kg-1)    Coef. eql. sorption on silt [0|1e9]
0.6               KClayEql_H      (L.kg-1)    Coef. eql. sorption on clay [0|1e9]
0.005             KOxEql_H        (L.mmol-1)  Coef. eql. sorption on oxides [0|1e9]
```

If the half-life is made dependent on soil type, the following parameters must be included in the substance specific section (see page 28 for further explanation):

```
* These parameters must be included to the corresponding compound section if DT50
* is calculated with a pedotransfer function (OptDT50 = Calculate).
* Replace pest by the appropriate compound name.
5.0               DT50Min_G       (d)         Minimum half-life
200.0             DT50Max_G       (d)         Maximum half-life
200.0             FacDT50Clay_G   (d)         Factor in PTF for DT50
100.0             FraClayDT50Ref_G    (-)     Reference clay content
1000.0            FacDT50Om_G     (d)         Factor in PTF for DT50
0.05              CntOmDT50Ref_G  (-)         Reference organic matter content
-2.0              FacDT50pH_G     (d)         Factor in PTF for DT50
7.0               pHDT50Ref_G     (-)         Reference pH
```

3.5 Adding and editing application schemes

Application schemes must be specified in the file with extension **app** (step 5 of 'Getting Started'). An example of this file is included in the examples directory. We recommend to make a copy of this file before editing. The applications file contains exactly the same information as the 'management' section of the PEARL input file as described in section 4.2.10. of

the FOCUS PEARL user manual. For detailed information on application schedules, the reader is referred to this manual.

Each application scheme starts with [scheme] and ends with [end_scheme], where scheme must be replaced by the actual name of the application scheme. Each section contains the following parameters:

- DelTimEvt: The application interval in years. Its value can be set to 1, 2 or 3. If set to 2, for example, biennial applications are simulated. Conform the FOCUS procedure (FOCUS, 2000), the simulation length (26, 46 or 66 years) is dependent on the value of this parameter.
- Table Applications: The applications table. The first columns contains the application date, the second column the application type, the third column the dosage and the fourth column the injection or tillage depth (if relevant). For further explanation of this table, see page 68 of the FOCUS PEARL manual. Please notice that in GeoPEARL only *user specified* interception fractions can be specified.
- Table TillageDates: Tillage events can be specified in the TillageDates table. The first column contains the date of tillage, the second column the tillage depth. See further page 68 of the FOCUS PEARL manual.

```
*-------------------------------------------------------------------------------
*
* Application schemes
*
* Column 1: Date
* Column 2: Application type: AppSolSur, AppSolInj, AppSolTil, AppCrpUsr
*
* If Type = AppSolSur (soil surface application):
* Column 3: Dosage (kg/ha) [0|-]
*
* If Type = AppSolInj (injection):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Injection depth (m) [0|-]
*
* If Type = AppSolTil (tillage):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Tillage depth (m) [0|-]
*
* If Type = AppCrpUsr (application to the crop canopy):
* Column 3: Dosage (kg/ha) [0|-]
* Column 4: Fraction of dosage applied to the crop canopy (-) [0|1]
*
*-------------------------------------------------------------------------------

*-------------------------------------------------------------------------------
* Aplication to the soil surface in spring

[springsurface]

1      DelTimEvt            Application interval

table Applications
26-May  AppSolSur 1
end_table

table TillageDates
end_table

[end_springsurface]
```

3.6 Editing the control file

All other changes for standard runs must be made in the **geo** file. An example of this file is in the root directory of GeoPEARL (i.e. the directory where GeoPEARL was installed). Make sure to make a copy before editing this file.

3.6.1 Specifying the input- and output directories

The directory where files are read or put can be changed. The position of files containing the executables must be specified in the BinDir record, the spatial schematisation must be specified in the SchematisationDir record, the position of the output files in the OutputDir record and temporary files are stored in the PearlDir. *Warning: if files are stored in a directory with spaces in its name, use relative paths only – otherwise GeoPEARL will not find these files.*

```
* Directory structure
* The input directory is obtained from the model call.
..\Bin              BinDir             Binary directory
..\Schematisation   SchematisationDir  Spatial schematisation
Output              OutputDir          Output directory
Tmp                 PearlDir           Tmp directory for PEARL runs
```

The following files can be put at any place:

- PlotListFile: file with plots to be simulated (page 47)
- CompoundProperties: file with substance properties (page 49)
- ApplicationSchemes: file with application schemes (page 49)
- OutputControl: output control file (page 50)

Therefore, the full path of these four files should be given at any time. The path name can, however, be relative to the position of the geo file (for example ..\examples\example.cmp).

3.6.2 Controlling the simulations

GeoPEARL has various options to control the simulation (step 6b of 'Getting Started').

- IOMode: Screen control. If set to 'IOMode_StdOut', screen output is limited and can be redirected to 'stdout', if wanted. If set to 'IOMode_Full', screen output is complete, but results cannot be captured to a text file.
- PriorityClass: Priority class for PEARL call. Can be set to Low, Normal or High. If GeoPEARL runs on a computer where you want run GeoPEARL in background, set PriorityClass to Low, otherwise choose a different option.
- OptAppend: OptAppend can have four values, i.e. 'Yes' , ' No' , ' SkipErrors' and 'New'
  - If set to 'Yes', results are appended to existing output files. If a plot has previously resulted in an error, a retry will be carried out.
  - If set to ' SkipErrors', results are appended to existing output files and plots that have previously resulted in an error will be ignored.
  - If set to 'No', new files will be created. Existing files with the same name will be replaced without further notice.
  - If set to ' New', new files will be created. If files exist already with the same name, GeoPEARL will give an error message.

- OptDelPloFiles: If set to 'Yes', GeoPEARL removes all temporary files when a plot is done (see the flow diagram in figure 11 of GeoPEARL report). This option should not be changed, unless you are testing the model.
- OptHyd: GeoPEARL can be used to simulate water balances only. Set OptHyd to Only to do so. See also page 61 of the FOCUS PEARL user manual.
- TimStart: The start-time of the simulations. For the Dutch registration procedure, TimStart should be 01-Jan-1901.
- TimEnd: The end-time of the simulations is dependent of the repeat interval of applications as specified in the applications file. It should be set to 31-Dec-1926 in the case of annual applications, 31-Dec-1946 in the case of biennial applications and 31-Dec-1966 in the case of triennial applications. See also page 60 of the FOCUS PEARL user manual.
- IniYears: The number of initialization years. These years or not used for the calculation of the percentiles of the annual leaching concentration. The value to be used in the registratoin procedure is 6.
- NumCPU: Maximum number of CPUs available for grid-computing. If GeoPEARL is used in a classical configuration, put NumCPU to 1. For further explanation of the grid-option, refer to section 3.11.
- CPUID: The CPU ID. If GeoPEARL is used in a classical configuration with one CPU only, put CPUID to 1. For further explanation of the grid option, refer to section 3.11.

```
*-------------------------------------------------------------------------------
* GeoPEARL control
*-------------------------------------------------------------------------------

IOMode_StdOut   IOMode                  Screen control [IOMode_Full|IOMode_StdOut]
Normal          PriorityClass           Priority class [Low|Normal|High]
Yes             OptAppend               Should files be appended?
Yes             OptDelPloFiles          Should the other plot files be removed?
Automatic       OptHyd                  SWAP mode: Automatic|OnLine|Only
01-Jan-1901     TimStart                Start time of the simulation
31-Dec-1926     TimEnd                  End time of simulation
6               InitYears               Number of years for initialization
1               NumCPU                  Number of CPUs for grid computing (1|-)
1               CPUID                   Number of the current CPU (1|NumCPU)
```

3.6.3 Plot selection

GeoPEARL has two options to select the plots to be included in the simulations, i.e. manually or automatically on the basis of the area of potential pesticide usage (i.e. area of the crop in which the substance is applied; see section 2.5 of GeoPEARL report). In the second case, plots are aggregated to larger computational units referred to as 'zones'. Selection between the two options of plot selection is done by setting the variable OptPlotList. The default in registration is 'Automatic'. If the user chooses for automatic plot selection, the results of the plot selection are written to a file extension with **crf**.

- OptPlotList has three options, i.e. 'Automatic', 'Manual' and 'Generate_Only':
  - If OptPlotList is set to 'Manual', the user must supply a file with plot numbers that must be included in the simulation. The name of this file (with extension **.lis**) should be specified in the record PlotListFile. Manual plot selection is particularly handy for testing as it makes it possible to run a single plot and check if the model runs well.

  - If OptPlotList is set to 'Automatic', the user must specify the crops for which a registration is requested (table Crops). You can chose between one of the crops included in table 2 of the GeoPEARL report. The user must specify three additional parameters, i.e. NumZone, ThresholdArea and OptPlotSelection.
  - If OptPlotList is set to 'Generate_Only', GeoPEARL will create a list with plot numbers to be included in the simulations, without actually starting the simulations. Results are written to a file with extension **crf**.
- CropAreaDataBase: The name of the file with information on crop areas per plot. The extension of this file is **unc**.
- NumZone: The number of zones. Although the minimum number of zones is 10, at least 250 zones must be used for reliable results (see chapter 4). Choosing a lower resolution should only be done when performing a quick-scan; runs with a low resolution are not accepted for the final registration.
- ThresholdArea: Plots with a crop area below this threshold are not included in the simulations. The default setting is 0.01 ha ha^{-1}.
- OptPlotSelection: Method for allocation of plots to zones. If option 'Rank' is chosen, plots are aggregated on the basis of their relative vulnerability index (see page 62). If option 'Neighbour' is selected, adjoining plots are put together. Option 'Rank' performs best for ordinary substances, otherwise the 'Neighbour' option should preferably be selected.
- SwapMisFile: In a number of cases, the SWAP model may not reach convergence. Plots where this happens are so-called 'swap missers' . These 'swap missers' can be specified in this file and are skipped.

```
*-------------------------------------------------------------------------------
* Reference to plot file and plots included in model run
*-------------------------------------------------------------------------------
holland         Plots                   Plot file (plo file, must be in plot directory)
Automatic       OptPlotList             Plot list: [Automatic|Manual|Generate_Only]

*-------------------------------------------------------------------------------
* If OptPlotList = Manual:
example         PlotListFile            File with plots to be simulated

*-------------------------------------------------------------------------------
* If OptPlotList = Automatic:
holland         CropAreaDatabase        Files with crop area per UC (unc file)
0.01            ThresholdArea   (ha)    Threshold area (0|-)
250             NumZone                 Number of zones (100|NumPlo)
Rank            OptPlotSelection        Option for plot selection [Neighbour|Rank]

* Crops for which a registration is submitted. The model takes the sum of the
* crop areas of the individual crops. Make sure that the name is exactly equal
* to one of the names in the crop area database.

table Crops
1  Potatoes
end_table

*-------------------------------------------------------------------------------
* SWAP missers - file must be put in schematisation directory
Swap207e              SwapMisFile             File with SWAP missers
```

3.6.4 Specification of compounds and applications to be included in the simulation

The final stage of editing consists of specifying the compounds and applications schemes that should be included in the simulations. There are three parameters that need to be edited:

- CompoundProperties: Full name (including directory name) of the file with substances properties. This file must have extension **cmp**. An example can be found in the examples directory.
- ApplicationSchemes: Full name of the file with application schemes. This file must have extension **app**. An example can be found in the examples directory.
- Table Runs: The first column of this table contains the substance name and the second column contains the application scheme to be included in the simulation. The following columns contain the code for each individual parent or daughter compound. Be sure that all names and codes match names and codes in the substances and applications files, respectively.

```
*-------------------------------------------------------------------------------
* Compound and application information
*-------------------------------------------------------------------------------

example    CompoundProperties    File with compound properties
example    ApplicationSchemes    File with application schemes

*-------------------------------------------------------------------------------
* Substances and application scheme. A run is made for each substance included
* Column 1  : Pesticide code - must be included in CompoundProperties file
* Column 2  : Application code - must be included in Applications file
* Column 3+ : Compound codes included in run (first = the daughter)

table Runs
NLA  springsurface NLA1 NLA2
end_table
```

3.6.5 Specification of the spatial schematisation

The following sections of the geo file contains references to the files with spatially distributed parameters. *In standard applications, these sections do not need editing.* References must be made to the soils file (SoilDatabase), the file with crop related evapotranspiration data (CropDatabase), the weather files (MeteoStations), the file with data on the lower boundary condition of SWAP (GroundwaterSystem) and the file with parameters of the local drainage system (DrainageSystem). The position of all these files must be specified in the SchematisationDir (see also page 46).

```
*-------------------------------------------------------------------------------
* Soil information (files must be stored in soil directory)

holland         SoilDatabase             Soil database

*-------------------------------------------------------------------------------
* Crop information (file must be stored in crops directory)

holland         CropDatabase             File with crop properties (extension crp)

*-------------------------------------------------------------------------------
* Information about meteo stations
* Column 1: ID
* Column 2: Latitude
* Column 3: Altitude (m)
```

```
* Column 4: Initial temperature (C)
* Column 5: Option for potential evapotranspiration
* ...       Input          : Reference evapotranspiration provided by user
* ...       Penman         : Penman reference evapotranspiration
* ...       Makkink        : Makkink reference evapotranspiration
* ...       PenmanMonteith : Penman Monteith evapotranspiration
* Column 6: Reference to the meteo file

table MeteoStations
1    52.0    10.0    9.97    Input  DeKooy
2    52.0    10.0    9.97    Input  Leeuwarden
3    52.0    10.0    9.97    Input  Eelde
4    52.0    10.0    9.97    Input  Hoorn
5    52.0    10.0    9.97    Input  Lelystad
6    52.0    10.0    9.97    Input  Dedemsvaart
7    52.0    10.0    9.97    Input  Naaldwijk
8    52.0    10.0    9.97    Input  DeBilt
9    52.0    10.0    9.97    Input  Winterswijk
10   52.0    10.0    9.97    Input  Andel
11   52.0    10.0    9.97    Input  Vlissingen
12   52.0    10.0    9.97    Input  Oudenbosch
13   52.0    10.0    9.97    Input  Gemert
14   52.0    10.0    9.97    Input  Venlo
15   52.0    10.0    9.97    Input  Beek
end_table

*-----------------------------------------------------------------------------
* Local and regional groundwater system
holland           GroundwaterSystem      Groundwater system (lbo file)
holland           DrainageSystem         Local drainage system (dra file)
```

3.6.6 Output and SWAP control

All other parameters of the geo file can be left at default values. As they are described in the FOCUS PEARL user manual (page 61 and 70), they are not discussed here.

```
*-----------------------------------------------------------------------------
* Output control data

Yes               OptScreen              Screen option (No|Swap_Only|Yes)
example           OutputControl          File with output data (ctr file)
Yes               PrintCumulatives       Print fluxes cumulative (Yes|No)
1.0               ZFoc            (m)    Depth of layer for balances
DaysFromSta       DateFormat             Format of dates in the output file
G12.4             RealFormat             Format of reals in the output file
Decade            OptDelTimPrn           Option for time step
1.0               DelTimPrn       (d)    Print time step - only if option is input

*-----------------------------------------------------------------------------
* SWAP control parameters

No                OptHysteresis               Simulate hysteresis?
1000000           MaxItSwa                    Maximum number of iterations
0.005             ThetaTol        (m3.m-3)    Tolerance for SWAP
1.d-5             DelTimSwaMin    (d)         Minimum time step for SWAP
0.20              DelTimSwaMax    (d)         Maximum time step for SWAP
1.0               GWLTol          (m)         Tolerance for groundwater level
```

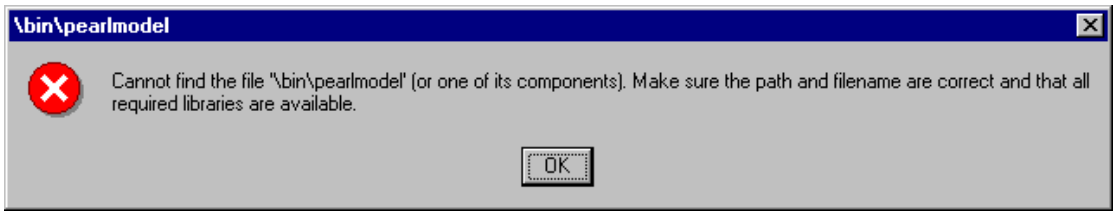
3.7 Running the model

Once all files have been edited, the model can be run. The command call consists of two parts; i.e. *the program name* and the *name of the run*. The name of the run is exactly the same as the name of the control file (the geo file). The full name *including the directory name*

should be specified here. The command can also be given from a command box or from the Total Commander© . After you have entered this command, the program will start. A flow-chart, which gives the order of the calculations, is given in figure 11 of the GeoPEARL manual. If you have set the option PriorityClass to Low, the program will run in background – you can then continue working on other projects without problems. During program execution, you should not log-off. If you use Windows XP, however, you may switch users. The program can be aborted any time by entering CNTRL-Break. If you have set OptAppend to Yes, you can restart where you ended.

3.7.1 Troubleshooting

- The following message appears:


\bin\pearlmodel
Cannot find the file '\bin\pearlmodel' (or one of its components). Make sure the path and filename are correct and that all required libraries are available.
OK

  Check if the call is correct. Did you give the proper directory name? Please remember that GeoPEARL and its components are in the bin directory.
- The program immediately terminates with the message 'Stop: Illegal run Id – no error file generated'. Check if the reference to the geo file is correct. Is the name correct? Is the directory correct? The program will also terminate if you have installed GeoPEARL in a directory that has a name with spaces.
- The program starts, but seems to stop immediately without further notice. In this case, get the error message from the error file and correct the error. The error file is in the output directory and has extension err.
- The program starts running PEARL. However, each PEARL run is stopped immediately and you will hear a large number of beeps. Handle as follows: Abort execution of GeoPEARL by typing CNTRL-Break. Read the error file and correct the problem(s). This problem is usually caused by errors in the substance or applications files. The best remedy to avoid errors in these files is to make copies of existing substances or application schemes and to make the changes in these copies.
- The program starts but does not actually perform any simulations. This is usually caused by the fact that OptAppend is set to Yes. Check if it is really necessary to make the simulations. Is all output already available? If not, set OptAppend to No or give the geo file another name to avoid conflicts with existing files.

3.8 Output files

GeoPEARL writes its results to a total number of nine output files, which are all stored in the output directory. The following files are generated (see also figure 18):

- Files with extension **wsb**. These files contain the annual and long-term average water balances of the soil profile.
- Files with extension **wfb**. These files contain the annual and long-term average water balances of the FOCUS layer. The thickness of the FOCUS layer is set by the variable ZFoc

in the output control section of the geo file. Following recommendations of the FOCUS working group (FOCUS, 2000), its default value is 1 m.

- Files with extension **csb**. These files contain the annual and long-term average substance balances of the soil profile.
- Files with extension **cfb**. These files contain the annual and long-term average substance balances of the FOCUS layer. The thickness of the FOCUS layer is set by the variable ZFoc in the output control section of the geo file. Following recommendations of the FOCUS working group (FOCUS, 2000), its default value is 1 m.
- Files with extension **ccb**. These files contain the annual and long-term average substances balances of the crop canopy.
- Files with extension **foc**. These files contain the percentiles of the leaching concentration at target depth. The target depth is set by the variable ZFoc in the output control section of the geo file. Following recommendations of the FOCUS working group (FOCUS, 2000), its default value is 1 m.
- Files with extension **day**. If detailed (daily) output is requested in the control file, results are written to these files. In standard applications, these files are empty.
- Files with extension **log**. This file contains the program log. You can review, for example, the computation times and see which plots have been done so far.
- Files with extension **err**. Error messages are written to these files.
- Files with extension **crf**. This files is generated if you have set OptPlotList to Automatic (page 47). This file gives the linkage between the zone numbers and the plot numbers and is needed when creating output maps.

3.8.1 The water balance of the individual plots (wsb and wfb files)

GeoPEARL gives, for each plot, the following annual and long-term average terms of the water balance (see also figure 20; the numbers refer to the column numbers in the files):

```
1  Plot          The plot number
2  Yr            The year or 'Avg' for long-term averages
3  DelLiq        Net storage change of water in profile       (m.a-1)
4  Prc           Precipitation                                (m.a-1)
5  Irr           Irrigation                                   (m.a-1)
6  FlvLea        Seepage at the lower boundary                (m.a-1)
7  FlvGrw        Groundwater recharge                         (m.a-1)
8  EvpInt        Evaporation of intercepted water             (m.a-1)
9  SolAct        Actual soil evaporation                      (m.a-1)
10 TrpAct        Actual transpiration                         (m.a-1)
11 Dra           Total discharge to drains and channels       (m.a-1)
12 Dra_1         Lateral discharge to primary system          (m.a-1)
13 Dra_2         Lateral discharge to secondary system        (m.a-1)
14 Dra_3         Lateral discharge to tertiary system         (m.a-1)
15 Dra_4         Lateral discharge to tube drains             (m.a-1)
16 Dra_5         Lateral discharge to surface drainage system (m.a-1)
17 Run           Run-off                                      (m.a-1)
18 EvpPnd        Evaporation of ponded water                  (m.a-1)
19 SolPot        Potential soil evaporation                   (m.a-1)
20 TrpPot        Potential transpiration                      (m.a-1)
```

The water balance is as follows and can be checked by importing the **wsb** and **wfb** files in a spreadsheet (for example EXCEL):

$$DelLiq = \Pr c + Irr - EvpInt - Run - SolAct - TrpAct - Dra - FlvLea \quad (1)$$

where *DelLiq* is the storage change. Please notify that the lower boundary flux, *FlvLea*, is negative if downwards. The groundwater recharge is calculated by integrating the flux over the phreatic groundwater table. In those cases where there is no local drainage system, this flux should be equal to the lower boundary flux (*FlvLea*).

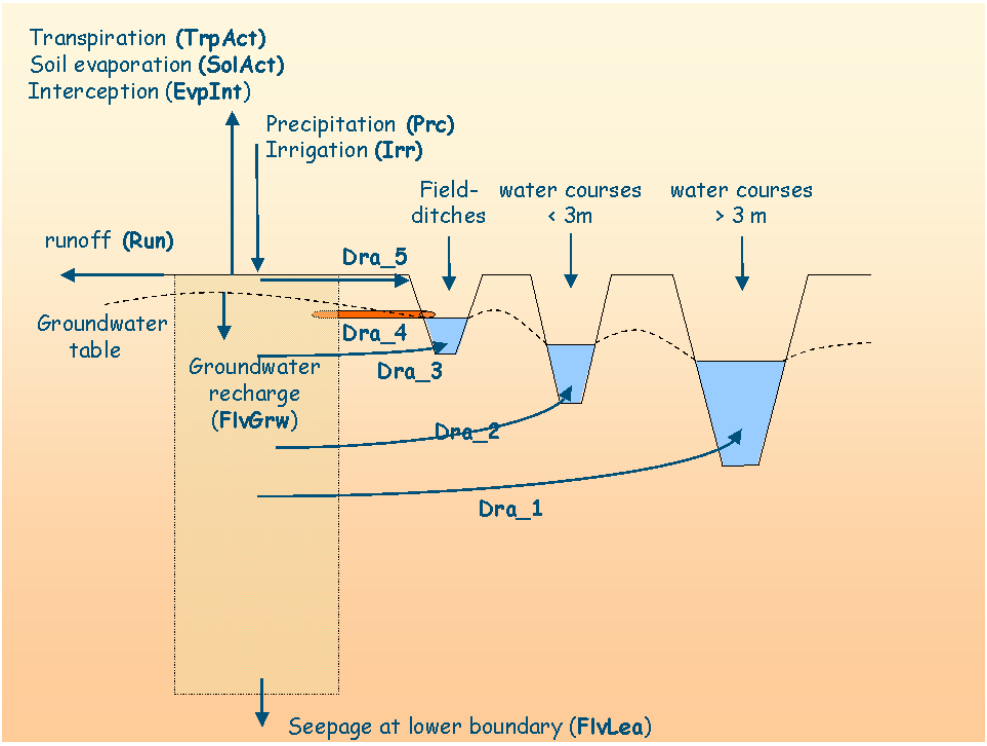


Figure 20. The GeoPEARL water balance

3.8.2 The substance balance of the individual plots (csb and cfb files)

Terms of the substance balance are given for all compounds (i.e. for both parents and metabolites). The **cfb** and **csb** contain the following columns (see also figure 21):

```
1  Plot          The plot number
2  Substance     Name of substance
3  Application   Name of application scheme
4  Yr            The year or 'Avg' for long-term averages
5  Cmp           Compound code
6  AmaAppSol     Areic mass applied to the soil system        (kg.ha-1.a-1)
7  DelAma        Change of mass in the soil system            (kg.ha-1.a-1)
8  DelAmaEql     Change of mass in the equilibrium domain     (kg.ha-1.a-1)
9  DelAmaNeq     Change of mass in the non-equilibrium domain (kg.ha-1.a-1)
10 AmaTra        Areic mass transformed in the soil system    (kg.ha-1.a-1)
11 AmaFor        Areic mass formed in the soil system         (kg.ha-1.a-1)
12 AmaUpt        Areic mass taken-up from the soil system     (kg.ha-1.a-1)
13 AmaDra        Areic mass drained from the soil system      (kg.ha-1.a-1)
14 AmaDra_1      Areic mass drained to the primary system     (kg.ha-1.a-1)
15 AmaDra_2      Areic mass drained to the secondary system   (kg.ha-1.a-1)
16 AmaDra_3      Areic mass drained to the tertiary system    (kg.ha-1.a-1)
17 AmaDra_4      Areic mass drained to tube drains            (kg.ha-1.a-1)
18 AmaDra_5      Areic mass drained to surface drain system   (kg.ha-1.a-1)
19 AmaDep        Areic mass deposited at the soil surface     (kg.ha-1.a-1)
20 AmaVol        Areic mass volatised from the soil surface   (kg.ha-1.a-1)
21 AmaLea        Areic mass leached from the soil system      (kg.ha-1.a-1)
22 AmaGrw        Areic mass leached into the deep aquifer     (kg.ha-1.a-1)
```

The substance balance is as follows and can be checked by importing the **csb** and **cfb** files in a spreadsheet (for example EXCEL):

$$DelAma = AmaApp + AmaDep - AmaVol - AmaLea - AmaUpt - AmaDra - AmaTra + AmaFor \quad (2)$$

where *DelAma* is the areic mass balance change. As with the water balances, net downward fluxes are negative.

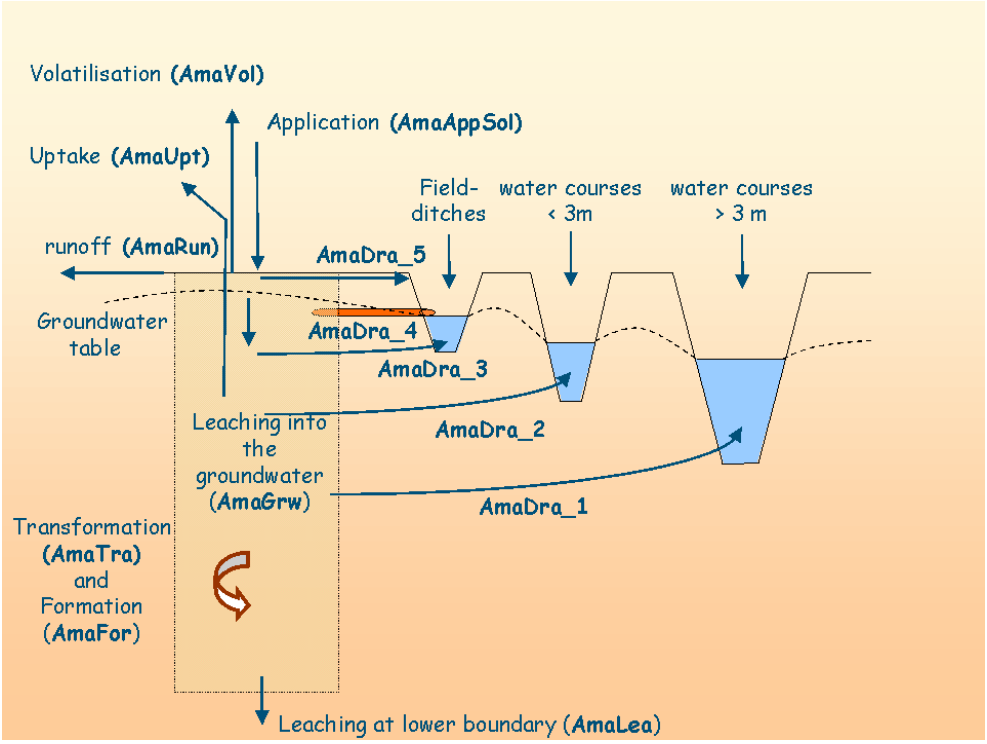


Figure 21.The GeoPEARL substance balance

3.8.3 Percentiles of the leaching concentration (foc file)

Percentiles in time of the mean annual leaching concentration at target depth are output to the file with extension **foc**. The default value for the target depth is 1 m and can be controlled by the variable ZFoc in the output control section of the geo file (page 50). For standard applications it should, however, not be changed. The calculation procedure for the percentiles is essentially the same as in the FOCUS procedure (FOCUS, 2000). To have correct percentiles generated, the simulation must conform to FOCUS requirements, which implies that:

- Repeated applications should be simulated by setting DelTimEvt in the control file to 1, 2 or 3 (page 45)
- The simulation length must be 26, 46 or 66 years, depending on the value of DelTimEvt. The simulation length is controlled by the variable TimEnd, which should be set to 31-Dec-1926, 31-Dec-1946 or 31-Dec-1966.
- The initialization period must be six years. The length of the initialization period is controlled by the variable IniYears (page 47).

The foc files contain the following columns:

```
1 Plot          The plot number
2 Substance     Name of substance
3 Application   Name of application scheme
4 Cmp           Compound code
5 Perc          Percentile with respect to weather conditions
6 Year          The year
7 ConLea        Leaching concentration at target depth            (ug.L-1)
```

In contrast to the European registration procedure, where 80th percentile of the leaching concentration is selected, *the target percentile for the Dutch registration procedure is the 50th percentile (i.e. the median value)*.

Link between zones and plots (crf file)

As specified before, GeoPEARL can aggregate plots to larger computational units called zones. Within each zone, the largest plot ('dominant plot') is assumed representative for the entire zone. Calculations are carried out for the dominant plot only. When making graphs or regional scale substance and water balances, the user needs a link between the zone number and the plot number. This link is given in the plot table of the crf file. The format of this file table is as follows:

```
1 Plot          The plot number
2 Zone          The zone number
3 Area          Area of plot
4 AreaCrop      Area of crop for which a registration is requested in plot
5 RelArea       Relative area of crop per plot (%)
```

3.8.4 Other output files

There are three additional output files:

- The **day** file, which contains detailed output. This file is only generated if additional output was requested by the user (page 50). The format of the **day** file is exactly the same as the format of the output file of FOCUS PEARL, so it is not further discussed here.
- The **log** file, which contains log information such as the computation time per plot.
- The **err** file, which contains error messages. If the model terminates normally, it should be empty.

3.9 The percentiles program

Summary reports, including the 90th percentile of the leaching concentration at the area of usage are generated by the percentiles program. To use this program, the following steps must be followed:

1. create an assessment file. This file must have the extension **.ass**;
2. edit this file. It is important to make a reference to all assessment items to get the appropriate 90th percentile;
3. run the program percentiles.exe;
4. results are written to a file with extension .per.

3.9.1 The assessment file

An example assessment file is listed below. An example is included in the example directory as well.

```
*-------------------------------------------------------------------------------
*
* Input file for the calculation of percentiles and maps of an assessment
* --> Initial version
*
1 ModelVersion  Model version
1 GUIVersion    GUI version
1 DBVersion     Database version
*-------------------------------------------------------------------------------
```

Percentiles.exe has the possibility to create maps of the 90th percentile of the leaching concentration. To use this option, set OptShowMaps to Yes. Maps have an automatic or predefined legend. This is controlled by the OptAutoScaling variable.

```
* General control parameters
No                  OptAppend              Append results to existing output files
Yes                 OptScreen              Screen output?
Yes                 OptShowMaps            Show the maps?
No                  OptAutoScaling         Auto scaling in maps (Yes|No)?
```

In the following section, you have to specify the directory structure. Both absolute and relative paths are possible.

```
* Directory to which the output file is written
output              OutputDir              Output directory
..\schematisation   SchematisationDir      Schematisation
..\bin              XYDir                  XY Directory
```

The next part refers to some basic maps. This section does not need editing.

```
* Map with unique combinations (must be in schematisation directory)
Holland_UC.map      UCMap                  Map with unique combinations
Holland.pol         Polygons               Map with country delineation
```

In this section, specify the assessment items that are part of the assessment. Please specify both the crop and the name of the file (including the path).

```
* Crops and files to be included in the assessment
* Both the crf and the foc files must be present
table Assessment
1 maize output\maize
2 potatoes output\potatoes
3 cereals output\cereals
end_table
```

3.9.2 Running the program

Once the assessment file has been edited, the program can be run. The command call consists of two parts; i.e. *the program name* and the *name of the assessment*. The name of the assessment is exactly the same as the name of the control file (the ass file). The full name *including the directory name* should be specified here. The command can also be given from a command box or from the Total Commander©.

3.9.3 Output of the program

The program gives three different tables:

- the leaching concentration for each zone included in the assessment. Zones are sorted on the basis of the leaching concentration;
- percentiles of the leaching concentration;
- the final summary, including the 90th percentile of the leaching concentration and the total area.

Notice that the overall percentiles are calculated for all items included in the assessment. If you want to calculate percentiles for a single crop, you have to create an assessment file with one crop.

3.10 Further output processing

On the basis of the obtained model outputs, the following results can be calculated:

- regional-scale substance and water balances;
- maps of terms of the water and substance balances;
- maps of the leaching concentration.

These results are not calculated by the current version of GeoPEARL but should be done by the user in a spreadsheet, database management system (DBMS) or a Geographical Information System (GIS). Notice that the GeoPEARL User Interface generates all these model outputs automatically.

The following actions could be followed to generate the wanted results (see also figure 22):

- First select the wanted model output from one of the output files. This can be done easily, as the output files are record oriented. To select the 50th percentile of the leaching concentration from the foc file, for example, simply select those records where column 5 has value 50. The actual selection can be done in a DBMS or spreadsheet.
- If you have chosen to run the model for a limited number of zones (with OptPlotList=Automatic), results in the output files are given per zone. The dominant plot number is then listed in the first column[1]. We suggest expanding these files to the full range of plots (i.e. list the results of all plots instead of a single plot per zone). This can be done with the information in the crf file, which contains the link between the zone number and the plot numbers. To do so, import the required output files in a spreadsheet or DBMS and perform a lookup operation with the dominant plot as the key variable (figure 22).

[1] This step may be skipped if you have run GeoPEARL for all plots (option OptPlotList=Manual).

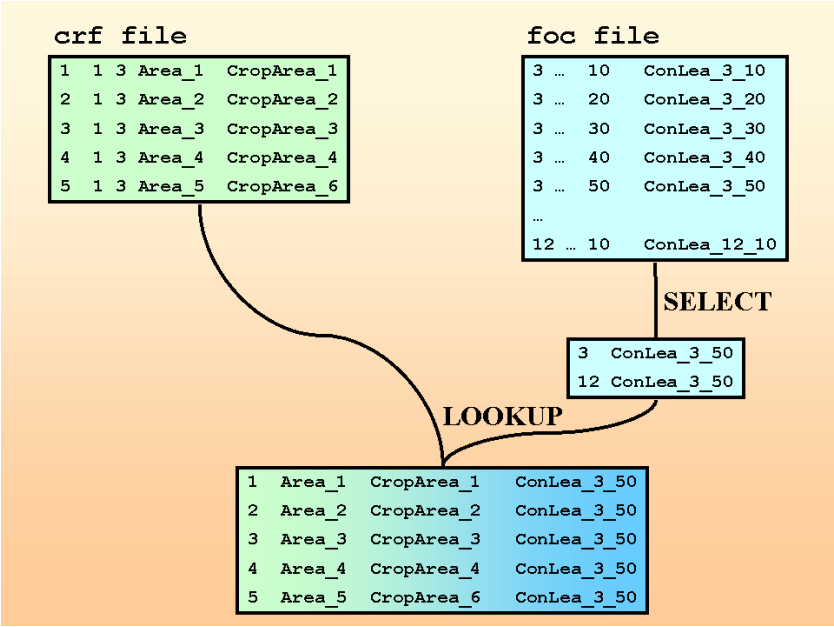


Figure 22.Diagram, which shows how to create tables for further processing.

- To create maps, the obtained table should be combined with the map of unique combinations. This map is called uc_holland_6405.map and is stored in the mapping directory of GeoPEARL. The map is in ASCIIGRID format and can be imported in many Geographical Information Systems, including ArcInfo™ and ArcView™.
- To present the concentration on the area of potential usage only, select only those plots where the relative crop area is above the threshold area as set in the geo file (variable ThresholdArea, page 47). The relative area (ha ha^{-1}) is calculated as the crop area in a plot (ha) divided by the total area of the plot (ha). The default value of the threshold value is 0.01 ha ha^{-1}.
- Maps of terms of the water and substance balances are created in a comparable way.
- Average substance and water balances and percentiles of the leaching concentration can be calculated from the obtained table, using the relative crop area as a weighing factor.

3.11 Using GeoPEARL on a grid

GeoPEARL can be used efficiently on a grid system, as the total simulation process can easily be split up in parts. An assessment with 6405 plots, for example, can be split-up in 100 ‘subruns’ and an acceleration factor of almost 100 will then be reached. To be able to run GeoPEARL on a grid system, the model has a number of features:

1. With the NumCPU parameter in the geo file, you can specify the number of computers that you have available in your grid. If, for example, you have 100 machines in your grid available, then enter a value of 100.
2. With the CPUID parameter, you can specify a subrun. Each subrun is assigned to a different computer on a grid. Consider the following example: The total number of plots in the assessment is 6405 (i.e. you want to run GeoPEARL for all plots in the schematisation). Presume that you have set NumCPU to 100, then the first subrun (CPUID=1) contains plot 1 to 64, the second subrun (CPUID=2) contains plots 65 to 128 and so on.

3. An alternative method to specify the CPUID is by using the command line:
   `geopearl example_1.geo /1` calls the first subrun
   `geopearl example_2.geo /2` calls the second subrun
   and so on.

Some tips when implementing GeoPEARL on a grid:

1. Create input files for an assessment (item), using the normal procedure described in section 3.1.
2. Specify the number of computer that you have available in the grid system. Use the Num-CPU in the geo file for this purpose (see above).
3. Copy all the input files to a shared directory, which is accessible from both the grid machines and from your local machine. You don't need to copy the input files to the grid machines (see figure 23).
4. Make sure that the binary directory (bin directory) is also a shared directory. You don't need to copy the binary files to the grid machines.
5. Make sure that the file references in the geo file refer to this shared directory. Also the output directory should be a shared directory and not a directory on the grid machine.
6. Keep the tmp directory on the grid machine to avoid too much network traffic.
7. You can now submit the GeoPEARL assessment to the grid. If the grid software that you are using has the possibility of submitting so-called job-arrays, then this is the way to submit. An example batch job for the LSF grid system is listed in section 3.11.1.
8. If all runs are ready, you have to merge the individual output files to one file. You get, for example, 100 files with extension .foc; they have to be merged to one file.
9. If done, you can run the percentiles program in a normal way.

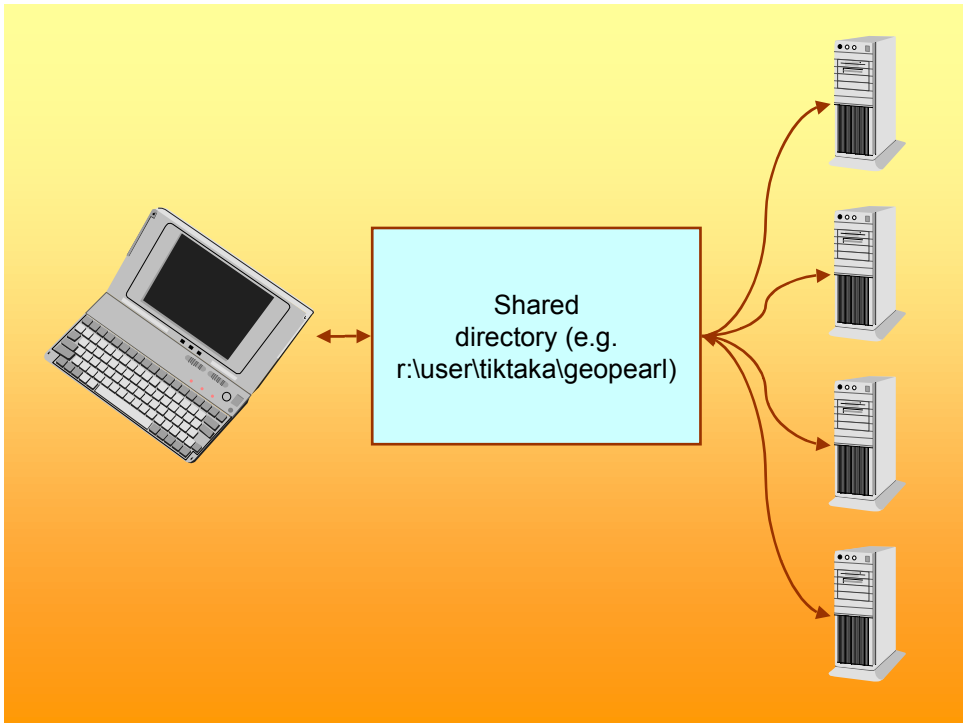


Figure 23. General set-up of a GeoPEARL grid implementation. To the right are the grid computers, to the left is your local machine.

3.11.1 Example for the platform™ LSF system

With the following command, you can submit a job with 100 subruns. The call uses the LSF bsub command, and calls a batch file, which is in a shared directory with the following name: r:\user\tiktaka\geopearl_1_1_1\run_pearl.cmd:

```
bsub -q pearl -J "pearl[1-100]" r:\user\tiktaka\geopearl_1_1_1\run_pearl.cmd
```

The batch file contains the following information:

```
@echo off

rem Directory on network drive
set GEODIR=r:\user\tiktaka\geopearl_1_1_1
echo %GEODIR%

echo Name of geofile (compd.geo)
set GEOFILE=compd
echo %GEOFILE%

rem Create output directory on network drive
if not exist %GEODIR%\%GEOFILE% mkdir %GEODIR%\%GEOFILE

rem Working directory on grid machine
rem Variable LSB_JOBID is automatically added by LSF. It is a unique number
rem added to avoid conflicts if more PEARL runs operate at the same grid machine
rem The local variable LSB_JOBINDEX is the number of subrun
set WORKDIR=%TEMP%\geopearl_1_1_1\%LSB_JOBID%\%LSB_JOBINDEX%
echo %WORKDIR%

rem Create working directory on remote machine
if not exist %WORKDIR% mkdir %WORKDIR%

rem Copy geo file. This is the only file that needs to be copied from the
rem network drive to the grid machine
copy %GEODIR%\%GEOFILE%.geo %WORKDIR%\%GEOFILE%%LSB_JOBINDEX%.geo

rem Execute GeoPEARL for one single job index
rem Model call expands to for example c:\localdrive\bin\geopearl compd1 /1
cd /d %WORKDIR%
%GEODIR%\bin\geopearl %GEOFILE%%LSB_JOBINDEX% /%LSB_JOBINDEX%

rem Clean up
cd ..
rmdir /s /q %WORKDIR%
```

For more information on the Platform LSF system, refer to www.platform.com.

4 Procedure for plot selection

As mentioned in chapter 2.3 of the GeoPEARL manual, the total run time of GeoPEARL is unacceptably long if all 6405 plots are included in a leaching assessment. The model therefore contains procedures to reduce the number of plots that must be included in a leaching study. Correct application of these procedures guarantee that the 90th percentile of the leaching concentration at the area of potential usage is hardly affected. This appendix describes the procedures and gives guidelines for correct application of these procedures.

4.1 Methodology

Reduction of the number of plots is done through a so-called 'slice' operation. During this operation, the total range of plots is sliced into a number of so-called zones that each *has an equal number of plots*. After having the slice operation completed, the plot with the largest area of potential usage (the dominant plot) is selected to represent the entire zone. Only those plots that are relevant for an assessment are included in the slice operation, which implies that only those plots are included at which the potential area of usage is unequal to zero. Consider the following example, in which a range of 18 relevant plots is sliced into five zones:

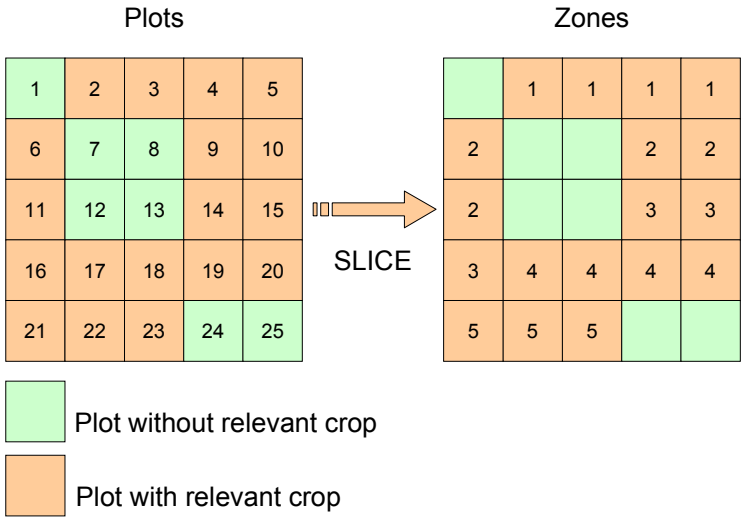


Figure 24. Slice operation performed on 18 relevant plots (see above). All plots in this example have a surface area of one single grid cell. Notice that the number of plots in each zone is between 3 and 4 due to rounding effects.

The minimum number of zones that should be included in a leaching study can be determined by analyzing the 90th percentile of the leaching concentration as a function of the number of zones. An efficient slice operation delivers a constant 90th percentile with few zones.

It may be expected that the efficiency of the slice operation will improve if zones are sampled in all classes of the cumulative frequency distribution of the leaching concentration. For this reason, a slice operation has been developed on the basis of the relative vulnerability to pesti-

cide leaching (further referred to as the *vulnerability index*). To get an a-priori estimate of the vulnerability index, the following procedure was followed:

1. For six ordinary behaving pesticides, the 50th percentile of the leaching concentration in time was simulated with GeoPEARL;
2. For each substance, the median leaching concentrations were scaled to the range 0 to 1;
3. For each plot, the average of the six so-obtained values was calculated
4. Each plot was assigned a relative ranking on the basis of its position at the cumulative frequency distribution.

4.2 Results

Results are shown in figure 25. Soils with low vulnerability are usually peat soils. The highest vulnerability is found in soils with a low organic matter content, such as dune and loess soils.

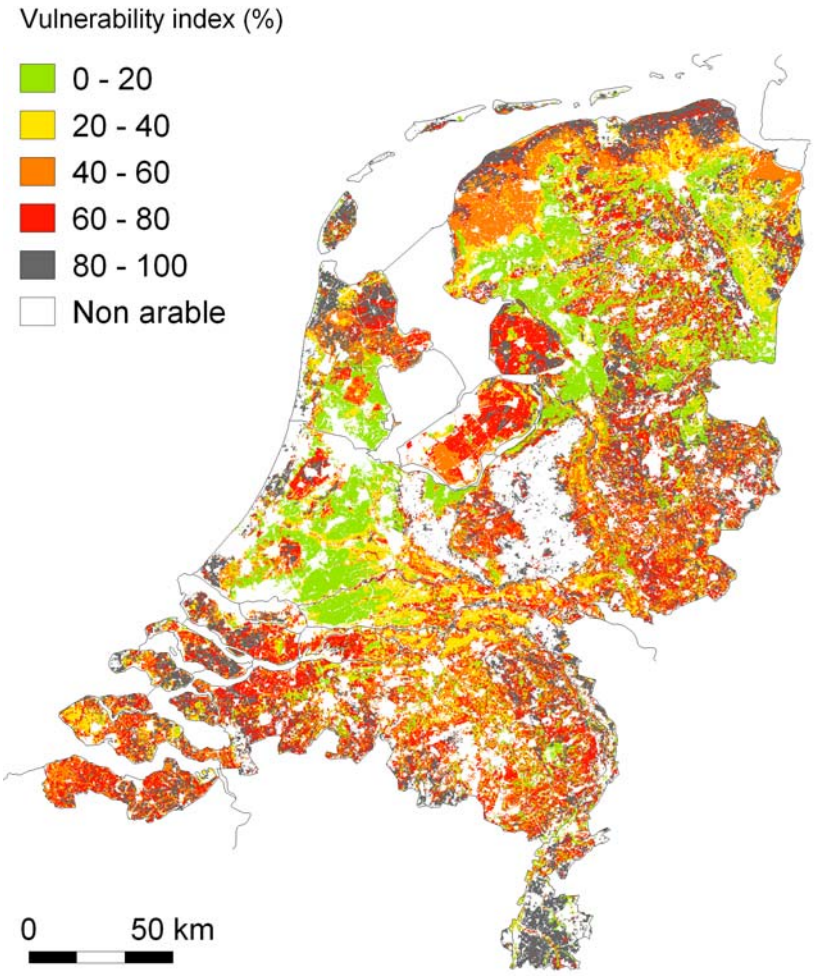


Figure 25. Vulnerability of soils to the leaching of ordinary behaving pesticides. Figures denote the class in the accumulated frequency distribution of the leaching concentration, for example 50% means that half of the soils are more vulnerable.

Figure 26 and 27 show the effect of the number of zones on the 90th percentile of the leaching concentration (PEC90). The first figure shows the effect of choosing a different crop, the sec-

ond figure shows the effect of different substances. Both figures show that, after an initial start, the fluctuations of the 90th percentile of the leaching concentration are generally small.

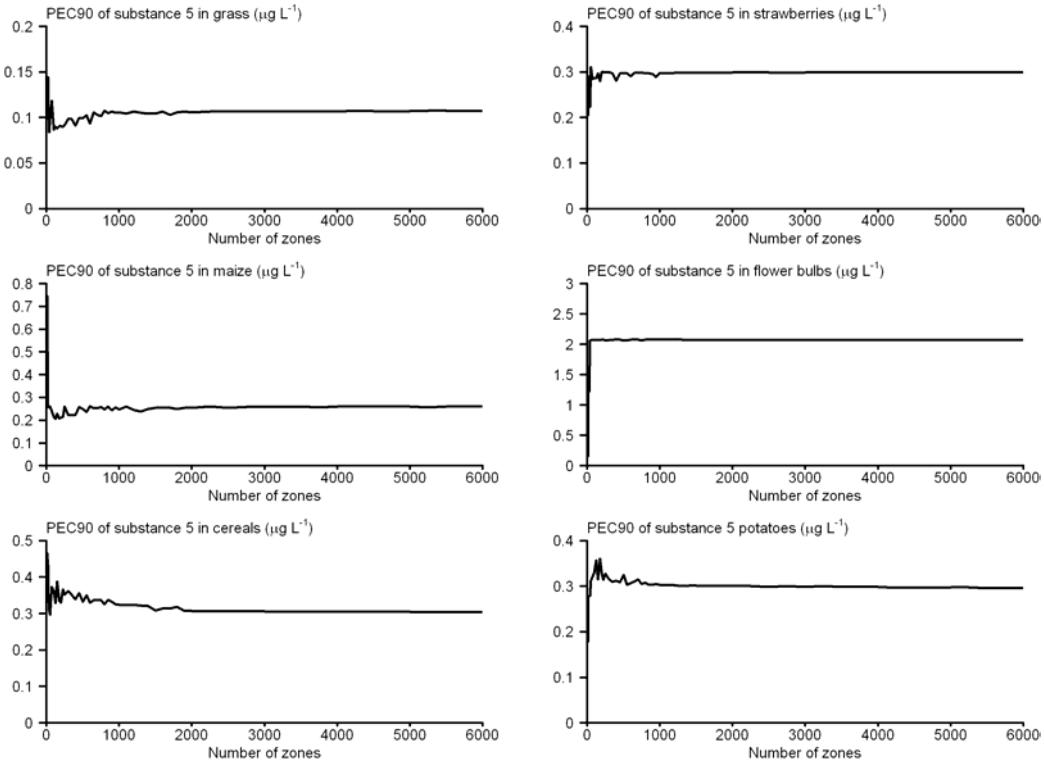

PEC90 of substance 5 in grass (µg L-1)
PEC90 of substance 5 in strawberries (µg L-1)
PEC90 of substance 5 in maize (µg L-1)
PEC90 of substance 5 in flower bulbs (µg L-1)
PEC90 of substance 5 in cereals (µg L-1)
PEC90 of substance 5 potatoes (µg L-1)
Number of zones

Figure 26. Effect of the number of zones on the 90th percentile of the leaching concentration at the area of potential usage.

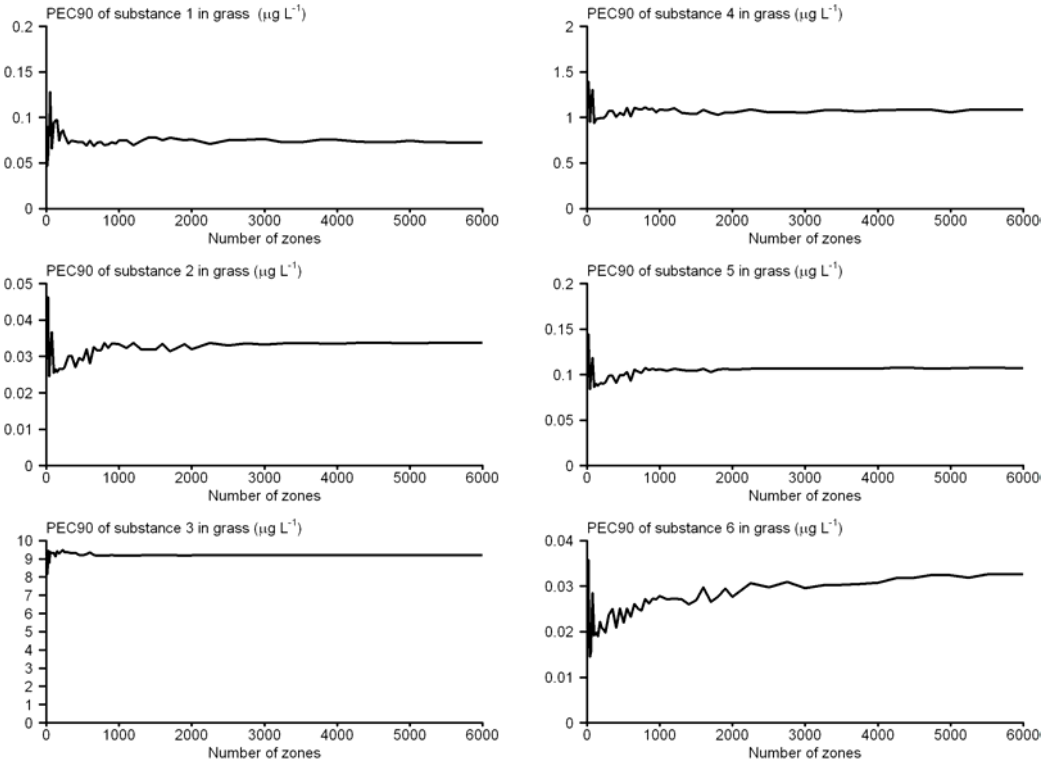

PEC90 of substance 1 in grass (µg L-1)
PEC90 of substance 4 in grass (µg L-1)
PEC90 of substance 2 in grass (µg L-1)
PEC90 of substance 5 in grass (µg L-1)
PEC90 of substance 3 in grass (µg L-1)
PEC90 of substance 6 in grass (µg L-1)
Number of zones

Figure 27. Effect of the number of zones on the 90th percentile of the leaching concentration at the area of potential usage.

The calculated spatial pattern of the leaching concentration is also remarkably stable, even if as few as 50 zones are included in the leaching assessment (figure 28). It can be concluded that the slice operation in GeoPEARL is extremely efficient in reducing the number of zones that are required in a leaching study. It should be noted, however, that the vulnerability index has been developed for ordinary behaving substances. Substances that show *p*H dependent sorption behavior should be treated with care.

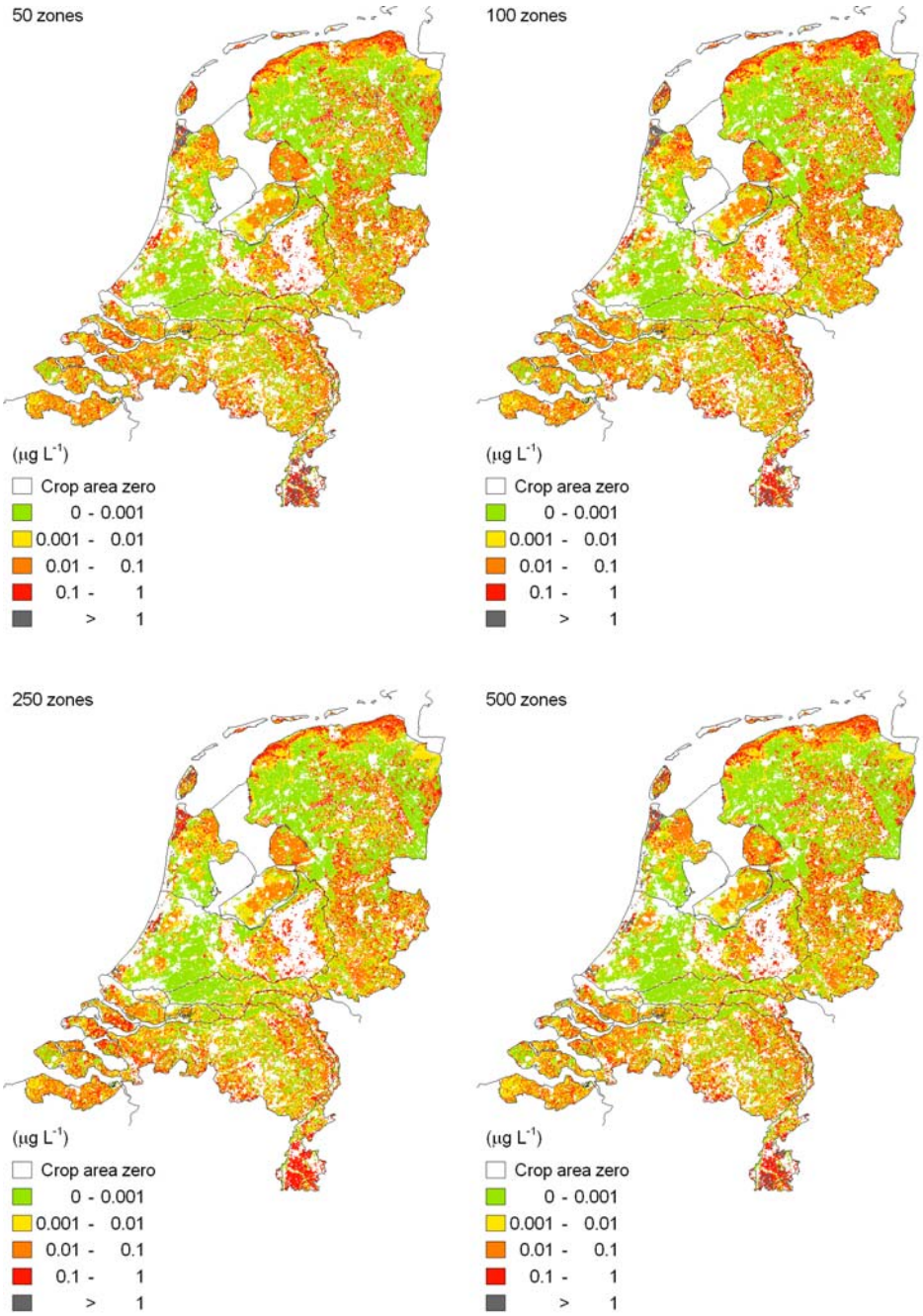


Figure 28. Effect of the number of zones on the predicted spatial pattern of the median leaching concentration for a hypothetical substance in grass.

5 Theory

5.1 Hydrology

Soil water flow

The SWAP model (Van Dam *et al*., 1997) uses a finite-difference method to solve the Richards equation:

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right] - R_{u,L} - R_{d,L} \tag{3}$$

where $C(h)$ (m^{-1}) is differential water capacity, t (d) is time, z (m) is vertical position, h (m) is soil water pressure head, $K(h)$ (m d^{-1}) is unsaturated hydraulic conductivity, $R_{u,L}$ (m^3 m^{-3} d^{-1}) is volumic volume rate of root water uptake, and $R_{d,L}$ (m^3 m^{-3} d^{-1}) is volumic volume rate of lateral discharge by drainage. SWAP can handle tabular data and analytical functions to describe the soil hydraulic properties. In the PEARL context, only the analytical equations proposed by Van Genuchten (1980) are supported:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1+(\alpha|h|)^n]^m} \tag{4}$$

and

$$K(h) = K_s S_e^{\lambda}\left[1-\left(1-S_e^{1/m}\right)^m\right]^2 \tag{5}$$

where θ_s (m^3 m^{-3}) is the saturated volume fraction of water, θ_r (m^3 m^{-3}) is the residual volume fraction of water, α (m^{-1}) reciprocal of the air entry value, K_s (m d^{-1}) saturated hydraulic conductivity, n (-) and λ (-) are parameters, m = 1-1/-n, and S_e (-) is the relative saturation, which is given by:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{6}$$

Potential evapotranspiration

The potential evapotranspiration, ET_p (m d^{-1}) is the key variable affecting the uptake of water by plant roots and soil evaporation. SWAP uses a slightly modified version of the Penman-Monteith equation (Monteith, 1965; Van Dam *et al*., 1997) to calculate the potential evapotranspiration. Recent comparative studies have shown a good performance of the Penman-Monteith approach under varying climatic conditions (Van Dam *et al.*, 1997). Potential and even actual evapotranspiration calculations are possible with the Penman-Monteith equation, through the introduction of canopy and air resistance's to water vapor diffusion. However, canopy and air resistance's may not be available. For this reason, SWAP follows a classical two step approach, i.e. (i) the calculation of the potential evapotranspiration, using the minimum value of the canopy resistance and the actual air resistance, and (ii) the calculation of the actual evapotranspiration using a reduction function. Application of the Penman-Monteith equation requires values of the air temperature, solar radiation, wind speed and air humidity. In SWAP, *daily* values of these parameters are used. See Van Dam *et al.* (1997) for details. SWAP calculates three quantities with the Penman-Monteith equation:

- ET_{w0} (m d^{-1}) potential evapotranspiration of a *wet* canopy, completely covering the soil
- ET_{p0} (m d^{-1}) potential evapotranspiration of a *dry* canopy, completely covering the soil
- E_{p0} (m d^{-1}) potential evaporation of a *wet,* bare soil.

As wind speed and air humidity are not always available, PEARL can alternatively calculate the reference evapotranspiration according to Makkink (1957), which requires daily values of temperature and solar radiation only. This equation, however, has some limitations: (i) it is developed for Dutch climatological conditions, and (ii) due to the lack of a ventilation term its performance in winter conditions is relatively poor. In this case, the potential evapotranspiration rate of a *dry* canopy, ET_{p0} (m d^{-1}) is calculated by:

$$ET_{p0} = f_c ET_r \tag{7}$$

where f_c (-) is an empirical crop factor, which depends on the crop type, and ET_r (m d^{-1}) is the reference evapotranspiration. Notice that this approach does not allow differentiation between a dry crop, a wet crop and wet soil. SWAP therefore assumes that these quantities are equal.

Potential transpiration and potential evaporation

The potential evapotranspiration is partitioned into the potential transpiration and the potential soil evaporation. The potential evaporation rate from a partly covered soil, E_p (m d^{-1}) is given by

$$E_p = \mathrm{e}^{-\kappa LAI} E_{p0} \tag{8}$$

where LAI (m^2 m^{-2}) is the Leaf Area Index, κ (-) is the extinction coefficient for global solar radiation, and E_{p0} (m d^{-1}) is the potential evaporation rate of a *wet* bare soil. As mentioned above, E_{p0} is equal to ET_{p0} if the Makkink equation has been used.

SWAP assumes that the evaporation rate of the water intercepted by the canopy is equal to ET_{w0}, independent of the soil cover fraction. The ratio of the daily amount of intercepted precipitation (see eqn. 14), P_i and ET_{w0} indicates the fraction of the day that the canopy is wet, f_w (-):

$$f_w = \frac{P_i}{ET_{w0}} \tag{9}$$

SWAP calculates a daily average of the potential transpiration rate, taking into account the fraction of the day that the canopy is wet (cf. Bouten, 1992):

$$T_p = (1 - f_w) ET_{p0} - E_p \qquad \text{with} \quad T_p \geq 0 \tag{10}$$

where T_p (m d^{-1}) is the potential transpiration rate in the case of a partly soil cover.

Uptake of water by plant roots

The maximum possible root water extraction rate, integrated over the rooting depth, is equal to the potential transpiration rate, T_p (m d^{-1}). The potential root water extraction rate at a given depth, $R_{u,L,p}(z)$ (m^3 m^{-3} d^{-1}), is calculated from the volumic root length, $L_{root}(z)$ (m m^{-3}) at that depth as a fraction of the integrated volumic root length (Tiktak and Bouten, 1992):

$$R_{u,L,p}(z) = \frac{L_{root}(z)}{\int_{z_{root}}^{0} L_{root}(z)\mathrm{d}z} T_p \tag{11}$$

Notice that SWAP does not account for preferential uptake from layers with high relative water saturation (Herkelrath *et al*., 1977; Tiktak and Bouten, 1992). The actual root water extraction rate, $R_{u,L}$, is calculated using a reduction function (Figure 29, Feddes *et al*., 1978):

$$R_{u,L}(z) = \alpha_w R_{u,L,p}(z) \tag{12}$$

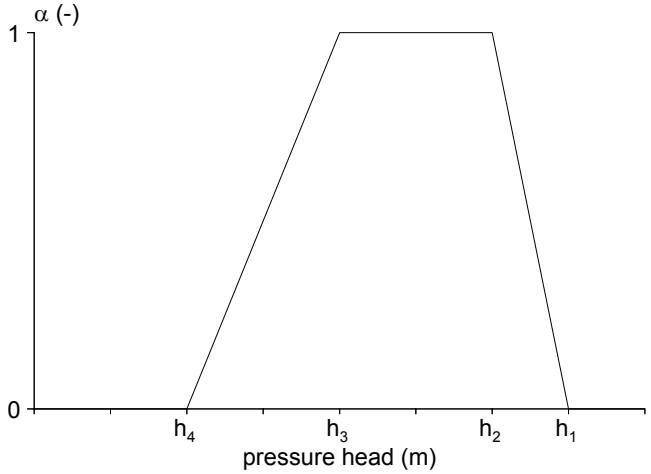


Figure 29 Reduction coefficient for root water uptake, α, as a function of soil water pressure head.

Evaporation of water from the soil surface

To calculate the actual soil evaporation rate, the potential soil evaporation rate is first limited to the maximum flux calculated from the Darcy equation for the top nodal point, E_{max}. The soil evaporation flux is additionally reduced according to the method proposed by Boesten and Stroosnijder (1986), who calculated the maximum actual soil evaporation, E_a (m) during a drying cycle:

$$\begin{aligned} \textstyle\sum E_a &= \textstyle\sum E_p \quad \text{if} \quad \sum E_p \le \beta^2 \\ \textstyle\sum E_a &= \beta\sqrt{\textstyle\sum E_p} \quad \text{if} \quad \sum E_p > \beta^2 \end{aligned} \tag{13}$$

where β ($m^{1/2}$) is an empirical parameter.

Interception of rainfall

Interception of rainfall by the crop canopy is calculated from the empirical equation (Braden, 1985):

$$P_i = a\,LAI\left[1 - \frac{1}{1 + (SC\,P)/(aLAI)}\right] \tag{14}$$

where P_i (m^3 m^{-2} d^{-1}) is intercepted precipitation, P (m^3 m^{-2} d^{-1}) is precipitation, SC (-) is the fraction of the soil covered by the crop, and a is an empirical parameter. In SWAP, the fraction of the soil covered by the crop is approximated by $LAI/3$ (Van Dam *et al*., 1997).

Bottom boundary conditions

SWAP makes a distinction between the local drainage flux to ditches and drains and the seepage flux due to regional groundwater flow. The seepage flux due to regional groundwater flow is the lower boundary flux (q_b), the local drainage flux is treated as a sink term ($R_{d,L}$). The following lower boundary conditions of SWAP can be used via the PEARL model*:*

1. Groundwater level, Φ_{gwl} (m), specified as a function of time.
2. Regional bottom flux q_b ($m^3\ m^{-2}\ d^{-1}$) specified as a function of time (Neumann condition).
3. Regional bottom flux is calculated using the hydraulic head difference between the phreatic groundwater and the groundwater in the semi-confined aquifer (pseudo two-dimensional Cauchy condition; Figure 30):

$$q_b = \frac{\Phi_{aqf} - \Phi_{avg}}{\gamma_{aqt}} \tag{15}$$

   where Φ_{aqf} (m) is hydraulic head of the semi-confined aquifer, Φ_{avg} (m) is average phreatic head, and γ_{aqt} (d) is vertical resistance of the aquitard. The average phreatic head is determined by the shape of the groundwater level in a field. The average phreatic head is calculated using the drainage base, Φ_d (m) and a shape-factor, β_{gwl}:

$$\Phi_{avg} = \Phi_d + \beta_{gwl}(\Phi_{gwl} - \Phi_d) \tag{16}$$

   Possible values for the shape factor are 0.64 (sinusoidal), 066 (parabolic), 0.79 (elliptic) and 1.00 (no drains present). Seasonal variation of the bottom flux can be induced through a sine-wave of the hydraulic head in the semi-confined aquifer.
4. q_b is calculated from an exponential flux-groundwater level relationship (Cauchy condition):

$$q_b = a_g e^{b_g|\Phi_{avg}|} \tag{17}$$

   with a_g (m d^{-1}) and b_g (m^{-1}) as empirical coefficients.
5. Pressure head of the bottom soil layer specified as a function of time (Dirichlet condition).
6. Zero flux at bottom of soil profile: $q_b = 0$ (special case of Neumann condition).
7. Free drainage of soil profile, in which case unit gradient is assumed at the lower boundary: $q_b = -K_{NumLay}$ (special case of Neumann condition).
8. Lysimeter boundary condition: Outflow only occurs if the pressure head of the bottom soil layer is above zero (special case of Neumann condition).

Lateral discharge of soil water

Lateral discharge rates can be calculated for a maximum number of five local drainage systems (e.g. drainage tiles and field-ditches). PEARL uses the following equation to calculate the flux to drainage system *k*:

$$q_{d,k} = \frac{\Phi_{avg} - \Phi_{d,k}}{\gamma_{d,k}} \tag{18}$$

where $q_{d,k}$ ($m^3\ m^{-2}\ d^{-1}$) is the flux of water to local drainage system *k*, $\Phi_{d,k}$ (m) is hydraulic head of drainage system *k*, and $\gamma_{d,k}$ (d) is drainage resistance. In order to distribute the discharge rates over the soil layers, first a discharge layer is determined by considering a travel-time distribution. The most important assumption in this computational procedure is that lateral discharge occurs to parallel, equidistant water courses (distance L_k (m)). See chapter 10.1

in Van Dam *et al*. (1997) for details. Within this discharge layer, the lateral drainage from soil layer *i* to local drainage system *k*, $R_{d,L,k,i}$, is calculated with the equation:

$$R_{d,L,k,i} = \frac{q_{d,k}}{\Delta z_i} \frac{K_{s,i}\Delta z_i}{\sum(K_{s,i}\Delta z_i)} \tag{19}$$

The total lateral drainage is calculated by summing the lateral drainage for all local drainage systems.

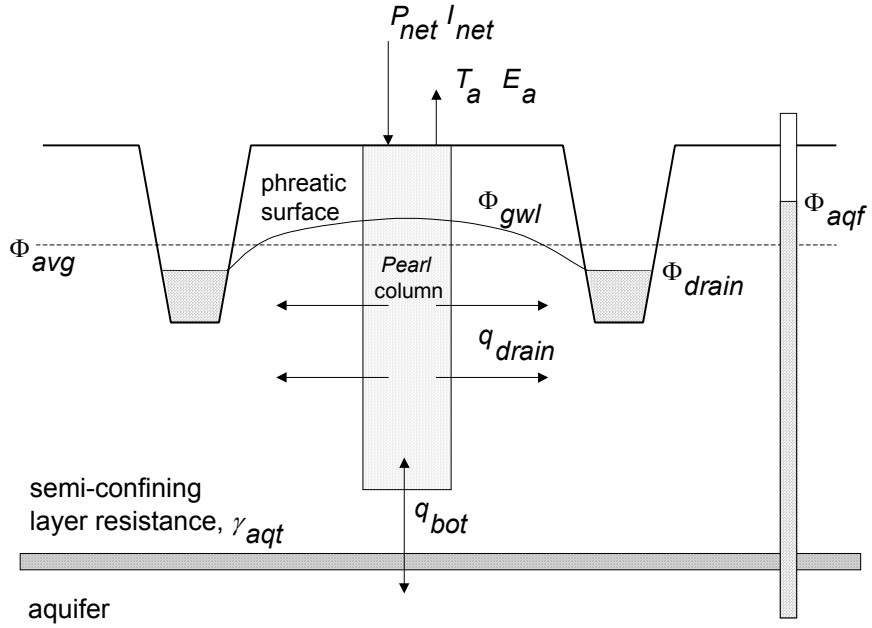


Figure 30 Pseudo two-dimensional Cauchy lower boundary condition, in case of drainage to ditches (Van Dam et al.*, 1997).*

5.2 Heat flow

The model SWAP (Van Dam *et al.*, 1997) calculates conductive transport of heat in soil:

$$\frac{\partial C_h T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda \frac{\partial T}{\partial z}\right] \tag{20}$$

where C_h (J m^{-3} K^{-1}) is the volumic heat capacity, T (K) is temperature, and λ (J m^{-1} d^{-1} K^{-1}) is the effective heat conductivity. The volumic heat capacity is calculated as the weighted mean of the heat capacities of the individual soil components (De Vries, 1963):

$$C_h = \theta_{sand} C_{sand} + \theta_{clay} C_{clay} + \theta_{om} C_{om} + \theta C_w + \varepsilon C_a \tag{21}$$

where θ_{sand}, θ_{clay}, θ_{om} and θ (m^3 m^{-3}) are the volume fractions of sand, clay, organic matter and water, ε (m^3 m^{-3}) is the air-filled porosity, and C_{sand}, C_{clay}, C_{om}, C_w and C_a (J m^{-3} K^{-1}) are the volumic heat capacities of the individual components. Table 1 gives an overview of the volumic heat capacity for the individual soil components. The volume fractions of sand, clay and organic matter are calculated from the mass percentages of sand, clay and organic matter, which are input to the model. The thermal conductivity is calculated according to the procedure described by Ashby *et al*. (1996), which accounts for both soil composition and soil geometry.

Table 1 Volumic heat capacity and thermal conductivity of the individual soil components (after Van Dam et al., 1997).

Component	Volumic heat capacity ($J\ cm^{-3}\ K^{-1}$)	Thermal conductivity ($J\ cm^{-1}\ K^{-1}\ d^{-1}$)
Sand	2.128	7603
Clay	2.385	2523
Organic matter	2.496	216
Water	4.180	492
Air (293 K)	1.212	22

The upper boundary condition for the soil heat-flow model is the daily average air temperature, T_{air} (K); the lower boundary condition is a zero-flux boundary condition. The heat flow equation is solved using a numerical method.

5.3 Pesticide fate

Pesticide application

Various factors affect the fraction of the dosage that is introduced into the soil system. During spraying, a fraction of the nominal dosage may be intercepted by the crop canopy. A part of the nominal dosage may drift from the field to adjacent ditches and fields. Another part may dissipate at the soil surface by processes like film volatilization and photochemical transformation. In PEARL, the user can choose from two general methods to describe the dosage introduced into the system:

1. Pesticide losses above the soil system are estimated beforehand, and the net load is introduced directly into the soil system.
2. The processes at the soil surface and plant surface are simulated in a simplified way.

Canopy processes

When a pesticide is sprayed on a field grown with plants, the nominal dosage has to be distributed over the plant canopy and the soil surface:

$$A_{d,p} = SC\ A_{d,f} \tag{22}$$

and

$$A_{d,s} = (1 - SC) A_{d,f} \tag{23}$$

where $A_{d,f}$ ($kg\ m^{-2}$) is the areic mass of pesticide applied to the field, $A_{d,p}$ ($kg\ m^{-2}$) is the areic mass of pesticide applied to the crop canopy, $A_{d,s}$ ($kg\ m^{-2}$) is the areic mass of pesticide deposited on the soil, and SC (-) is the fraction of the soil surface covered by the crop. All areic masses are expressed per m^2 field surface. Methods are being developed for more targeted spraying on plants or on the soil surface, so the soil cover fraction may not be appropriate. In this particular case, the fraction of the dosage that is deposited onto the crop canopy can be introduced by the user.

The following processes are described at the plant surface: (i) volatilization into the air, (ii) penetration into the plant, (iii) transformation at the plant surface, and (iv) wash-off via rainfall. The first three processes are described by first-order kinetics:

$$R_{dsp} = k_{v,p} A_p + k_{p,p} A_p + k_{t,p} A_p \quad (24)$$

where R_{dsp} (kg m^{-2} d^{-1}) is the areic mass rate of dissipation of pesticide at the plant surface, $k_{v,p}$ (d^{-1}) is rate coefficient for volatilization, $k_{p,p}$ (d^{-1}) is rate coefficient for penetration, $k_{t,p}$ (d^{-1}) is rate coefficient for transformation at the plant surface, and A_p (kg m^{-2}) is areic mass of pesticide at the crop canopy. Alternatively, the user can introduce an overall dissipation rate coefficient, k_{dsp} (d^{-1}) for the three processes. The areic mass rate of pesticide wash-off is taken proportional to the canopy drip flux:

$$R_{w,p} = w_p (SC\ P - P_i) A_p \quad (25)$$

where $R_{w,p}$ (kg m^{-2} d^{-1}) is the areic mass rate of pesticide wash-off from the crop canopy, w_p (m^{-1}) is an empirical wash-off factor, P (m d^{-1}) is precipitation, and P_i (m d^{-1}) is intercepted water. The following mass balance applies for the crop canopy:

$$\frac{\partial A_p}{\partial t} = -R_{w,p} - R_{dsp} \quad (26)$$

Mass balance equations

Pesticide can be found in the equilibrium domain and in the non-equilibrium domain of the soil system, so two mass balances apply:

$$\frac{\partial c^*_{eq}}{\partial t} = -R_s - \frac{\partial J_{p,L}}{\partial z} - \frac{\partial J_{p,g}}{\partial z} - R_t + R_f - R_u - R_d \quad (27)$$

and

$$\frac{\partial c^*_{ne}}{\partial t} = R_s \quad (28)$$

Here, c^*_{eq} (kg m^{-3}) is the pesticide concentration in the equilibrium domain of the soil system, c^*_{ne} (kg m^{-3}) is the pesticide concentration in the non-equilibrium domain of the soil system, R_s (kg m^{-3} d^{-1}) is the volumic mass rate of pesticide sorption, $J_{p,L}$ (kg m^{-2} d^{-1}) is the mass flux of pesticide in the liquid phase, $J_{p,g}$ (kg m^{-2} d^{-1}) is the mass flux of pesticide in the gas phase, R_t (kg m^{-3} d^{-1}) is the transformation rate, R_f (kg m^{-3} d^{-1}) is the formation rate, R_u (kg m^{-3} d^{-1}) is the rate of pesticide uptake by plant roots, and R_d (kg m^{-3} d^{-1}) is the lateral discharge rate of pesticides.

Transport in the liquid phase

Transport of the pesticide in the liquid phase of the soil is described by an equation including convection, dispersion and diffusion:

$$J_{p,L} = q c_L - D_{dis,L} \frac{\partial c_L}{\partial z} - D_{dif,L} \frac{\partial c_L}{\partial z} \quad (29)$$

where $J_{p,L}$ (kg m^{-2} d^{-1}) is the mass flux of pesticide in the liquid phase, q (m^3 m^{-2} d^{-1}) is the soil water flux, $D_{dis,L}$ (m^2 d^{-1}) is coefficient of pesticide dispersion in the liquid phase, z (m) is vertical position, and $D_{dif,L}$ (m^2 d^{-1}) is the coefficient of pesticide diffusion in the liquid phase. The dispersion coefficient is taken to be proportional to the soil water flux:

$$D_{dis,L} = L_{dis,L} |q| \quad (30)$$

with $L_{dis,L}$ (m) as the dispersion length. The diffusion of pesticide in the liquid phase is described by Fick's law. The coefficient for diffusion of pesticide in the liquid phase is calculated by:

$$D_{dif,L} = \zeta_L D_w \tag{31}$$

where ζ_L (-) is the relative diffusion coefficient in the liquid phase, and D_w ($m^2\ d^{-1}$) is the coefficient of pesticide diffusion in pure water.

The relative diffusion coefficient is a function of the volume fraction of liquid. PEARL offers three methods do describe this function. By default, the function proposed by Millington and Quirk (1960) is used:

$$\zeta_L = \theta^{a_{M,L}} / \theta_s^{b_{M,L}} \tag{32}$$

where θ ($m^3\ m^{-3}$) is the volume fraction of liquid, θ_s ($m^3\ m^{-3}$) is the volume fraction of liquid at saturation, and $a_{M,L}$ (-) and $b_{M,L}$ (-) are empirical parameters. The second type of equation is the one used by Currie (1960):

$$\zeta_L = a_{C,L}\theta^{b_{C,L}} \tag{33}$$

where $a_{C,L}$ (-) and $b_{C,L}$ (-) are empirical coefficients. The third equation is suggested by Troeh *et al.* (1982). In this approach, diffusion in the liquid phase is taken to be zero in a range of (low) volume fractions of water. In this range, the water-filled pores are assumed to be discontinuous:

$$\zeta_L = \begin{cases} \left(\dfrac{\theta - a_{T,L}}{1 - a_{T,L}}\right)^{b_{T,L}} & \text{if} \quad \theta > a_{T,L} \\ 0 & \text{if} \quad \theta \le a_{T,L} \end{cases} \tag{34}$$

where $a_{T,L}$ ($m^3\ m^{-3}$) is the volume fraction of water at the air-entry point, and $b_{T,L}$ (-) is an empirical parameter.

The value of the diffusion coefficient in water is temperature dependent, mainly because the viscosity of water depends on the temperature. In PEARL, the theoretically derived Stokes-Einstein equation (Tucker and Nelken, 1982) is approximated by:

$$D_w = 1 + 0.0257\left(T - T_r\right)D_{w,r} \tag{35}$$

where T (K) is temperature, T_r (K) is reference temperature, and $D_{w,r}$ ($m^2\ d^{-1}$) is the diffusion coefficient in water at reference temperature. See Leistra *et al*. (2000) for details.

Transport in the gas phase

Transport of pesticide in the gas phase is described by Fick's law:

$$J_{p,g} = -D_{dif,g}\frac{\partial c_g}{\partial z} \tag{36}$$

where $J_{p,g}$ ($kg\ m^{-2}\ d^{-1}$) is mass flux of pesticide in the gas phase, and $D_{dif,g}$ ($m^2\ d^{-1}$) is coefficient of pesticide diffusion in the gas phase. The coefficient for diffusion of pesticide in the gas phase is calculated by:

$$D_{dif,g} = \zeta_g D_a \tag{37}$$

where ζ_g (-) is the relative diffusion coefficient in the gas phase, and D_a (m^2 d^{-1}) is the coefficient of pesticide diffusion in air. The relation between D_a and temperature is described by:

$$D_a = \left(\frac{T}{T_r}\right)^{1.75} D_{a,r} \tag{38}$$

where $D_{a,r}$ (m^2 d^{-1}) is the diffusion coefficient in air at reference temperature. The relative diffusion coefficient is a function of the volume fraction of the gas phase. It is calculated analogous to the relative diffusion coefficient in the liquid phase (eqn. 32-34).

Initial and boundary conditions

The initial condition for the model is defined by profiles of the concentration of pesticide in the equilibrium domain of the soil system, c^*_{eq} (kg m^{-3}), and in the non-equilibrium domain of the soil system, c^*_{ne} (kg m^{-3}). It is further assumed that at the start of the simulation the areic mass of pesticide at the plant surface, A_p, is zero.

The boundary condition at the soil surface is a flux boundary condition. The user can enter deposition fluxes of pesticide as a function of time. Pesticides entering the system by deposition are subject to canopy processes. The user can also specify the concentration of pesticide in irrigation water, in which case the user has to choose between surface irrigation (i.e. application of irrigation water directly to the soil system) and sprinkler irrigation (application to the crop canopy).

At the lower boundary of the soil system, dispersive and diffusive fluxes of pesticide are assumed to be zero. In the case of infiltration of water from a deep aquifer, the pesticide concentration is set to zero.

Diffusion of pesticide vapor in the gas phase of the soil is included in the model, which implies that a description of pesticide volatilization at the soil surface is required. In the current model version, the diffusion of vapor through the soil and a laminar air-boundary layer are the limiting factors for volatilization (cf. Jury *et al.*, 1990):

$$J_{p,v} = \frac{c_g}{r_{s,v} + r_{a,v}} \tag{39}$$

where $J_{p,v}$ (kg m^{-2} d^{-1}) is the mass flux of pesticide volatilization, c_g (kg m^{-3}) is concentration of pesticide in the gas phase of the top layer, $r_{s,v}$ (d m^{-1}) is resistance of the soil boundary layer, and $r_{a,v}$ (d m^{-1}) is resistance of the air boundary layer. The resistance's of the boundary layers are calculated by:

$$r_{s,v} = \frac{d_s}{D_{dif,g}} \qquad \text{and} \qquad r_{a,v} = \frac{d_a}{D_a} \tag{40}$$

where d_s (m) is thickness of soil boundary layer, $D_{dif,g}$ (m^2 d^{-1}) is the coefficient for diffusion of pesticide in the gas phase of the soil system, d_a (m) is the thickness of the laminar air-boundary layer, and D_a (m^2 d^{-1}) is coefficient for diffusion of pesticide in air. It should be noted that the current description of pesticide volatilization is subject to considerable uncertainty, particularly for surface-applied pesticides where initial volatilization is hardly limited by the soil boundary layer. For this reason, at present research aimed at improving the sub-

model for pesticide volatilization is being carried out. See Leistra *et al*. (2000) for further considerations.

Partitioning over the three soil phases

The sorption of pesticide on the soil solid phase is described with a Freundlich equation. Both equilibrium and non-equilibrium (kinetic) sorption are considered. Equilibrium sorption is described by the equation:

$$X_{eq} = K_{F,eq} c_{L,r} \left(\frac{c_L}{c_{L,r}} \right)^N \tag{41}$$

in which X_{eq} (kg kg^{-1}) is pesticide content in the equilibrium sorption phase, $K_{F,eq}$ (m^3 kg^{-1}) is Freundlich coefficient for the equilibrium-sorption phase, c_L (kg m^{-3}) is concentration in the liquid phase, $c_{L,r}$ (kg m^{-3}) is reference concentration in the liquid phase and N is the Freundlich exponent. Notice that a particular type of Freundlich equation is used in the model, by introducing the reference concentration. The advantage of this type of equation is that the unit of the Freundlich coefficient becomes independent of the exponent.

The Freundlich coefficient may depend on various soil properties, such as organic matter content, oxide content and pH. For most pesticides, the following equation is appropriate:

$$K_{F,eq} = m_{om} K_{om,eq} \tag{42}$$

where m_{om} (kg kg^{-1}) is mass content of organic matter in soil and $K_{om,eq}$ (m^3 kg^{-1}) is the coefficient of equilibrium sorption on organic matter.

PEARL contains a description of the sorption of weak acids, which is *p*H dependent:

$$K_{F,eq} = m_{om} \frac{K_{om.\mathrm{eq,ac}} + K_{om,eq,ba} \dfrac{M_{ba}}{M_{\mathrm{ac}}} 10^{p\mathrm{H}\text{-}p\mathrm{Ka}\text{-}\Delta p\mathrm{H}}}{1 + \dfrac{M_{ba}}{M_{\mathrm{ac}}} 10^{\mathrm{pH}\text{-}p\mathrm{Ka}\text{-}\Delta p\mathrm{H}}} \tag{43}$$

where $K_{om,\mathrm{eq,ac}}$ (m^3 kg^{-1}) is the coefficient for sorption on organic matter under acidic conditions, $K_{om,eq,ba}$ (m^3 kg^{-1}) is the coefficient for sorption on organic matter under basic conditions, M (kg mol^{-1}) is molar mass, *p*Ka is the negative logarithm of the dissociation constant, and Δ*p*H is a *p*H correction factor. See Leistra et al. (2000) for the derivation of this equation.

At low *p*H values, sorption is dominated by the neutral molecule; the exponent in equation 43 becomes negative, almost eliminating the second term at the right-hand side while the denominator approaches one. In contrast, at high *p*H values, the denominator becomes large, thereby eliminating the contribution of the neutral molecule. The anions are repelled by the negative charge of the surfaces of organic matter and clay minerals, so sorption is often low. However, the anions may show some residual sorption due to hydrophobic interactions between a more hydrophobic part of the molecule and organic matter. Equation 43 can also be used for weak bases, where the protonated species is more strongly sorbed than the neutral molecule. In equation 43, an additional term Δ*p*H or *p*H-shift is included to account for discrepancies between experimental conditions in sorption tests and the conditions for which one wants to calculate the leaching of a substance. The *p*H of the soil is dependent on the way it is

measured. Several methods exist, of which the most obvious differences between the methods are the composition and the concentration of the solution used to prepare the slurry, usually H_2O, KCl or $CaCl_2$. It is likely that the concentration of exchangeable cations and the way in which the *p*H is measured affect the *p*H-value obtained.

The sorption of some pesticides cannot be described with the organic matter equilibrium constant. This is particularly true for those pesticides that sorb preferentially on clay and oxides. FOCUS PEARL 2.2.2. has an option to make the sorption dependent on depth:

$$K_{F,eq} = f_{d,s} K_{F,eq,r} \tag{44}$$

where $K_{F,eq,r}$ ($m^3\ kg^{-1}$) is the Freundlich coefficient in the topsoil, and $f_{d,s}$ (-) is an empirical depth-effect factor. In the case of GeoPEARL, this option is not practical as the depth dependence of sorption should be specified for each individual soil profile included in the simulations. Therefore, an option is included in GeoPEARL to relate the sorption to other soil characteristics than organic matter. For the moment this option is restricted to parameters that are available in the soil database distributed with GeoPEARL (i.e. soil texture, soil organic matter and sesqui-oxide content). The overall sorption is described with an equation analogous to equation 42:

$$K_{F,eq} = K_{F,eq,0} + m_{om} K_{om,eq} + m_{sand} K_{sand,eq} + m_{silt} K_{silt,eq} + m_{clay} K_{clay,eq} + c_{sox} K_{sox,eq} \tag{45}$$

where $K_{F,eq}$ ($m^3\ kg^{-1}$) is the overall Freundlich sorption coefficient, $K_{F,eq,0}$ ($m^3\ kg^{-1}$) is the Freundlich equilibrium sorption coefficient for sorption not attributable to a particular soil parameter, m_{om} ($kg\ kg^{-1}$) is the mass fraction of organic matter, $K_{om,eq}$ ($m^3\ kg^{-1}$) is the coefficient for sorption on organic matter, m_{sand}, m_{silt} and m_{clay} ($kg\ kg^{-1}$) are the mass fractions of sand, silt and clay, $K_{sand,eq}$, $K_{silt,eq}$ and $K_{clay,eq}$ ($m^3\ kg^{-1}$) are the coefficients for sorption on sand, silt and clay, respectively, c_{sox} ($mmol\ kg^{-1}$) is the soil content of sesqui-oxides and $K_{sox,eq}$ ($m^3\ mmol^{-1}$) is the coefficient for sorption on sesqui-oxides. Notice that the textural distribution must be expressed as parts of the mineral soils, so that the sum of sand, silt and clay is equal to one.

The assumption is that the sorption is linearly related to the content of each soil parameter. If the content or fraction of a specific soil characteristic is zero, then there is no contribution. If, for example, only sorption onto sand is to be simulated, equation 45 reduces to:

$$K_{F,eq} = m_{sand} K_{sand,eq} \tag{46}$$

Pesticide sorption to the non-equilibrium phase is described by a first-order rate equation:

$$R_s = \rho_b k_d \left[f_{K,ne} K_{F,eq} c_{L,r} \left(\frac{c_L}{c_{L,r}} \right)^N - X_{ne} \right] \tag{47}$$

where R_s ($kg\ m^{-3}\ d^{-1}$) is rate of sorption in the non-equilibrium domain of the soil system, ρ_b ($kg\ m^{-3}$) is the dry bulk density of the soil, X_{ne} ($kg\ kg^{-1}$) is pesticide content at non-equilibrium sorption sites, k_d (d^{-1}) is desorption rate coefficient, and $f_{K,ne}$ (-) is factor describing the ratio $K_{F,ne}/K_{F,eq}$, with $K_{F,ne}$ ($m^3\ kg^{-1}$) as the Freundlich coefficient for the non-equilibrium sorption phase. See Leistra *et al*. (2000) for a discussion of the theoretical background of this equation.

The effect of temperature on both the equilibrium and the non-equilibrium Freundlich coefficient is described with

$$K_{F,eq} = K_{F,eq,ref} \exp\left[\frac{-\Delta H_s}{R}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right] \quad (48)$$

$$K_{F,ne} = K_{F,ne,ref} \exp\left[\frac{-\Delta H_s}{R}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right] \quad (49)$$

in which the subscript *ref* indicates a reference temperature and in which ΔH_s is the molar enthalpy of sorption (J mol^{-1}). The default value of ΔH_s is 0 (no effect of temperature on sorption). Usually the Freundlich coefficients decrease with increasing temperature (Calvet *et al.*, 1980), which implies that ΔH_s is negative. However, sometimes positive values of ΔH_s have been found (Dao and Lavy, 1978; Boesten and Van der Pas, 2000).

The partitioning of the pesticide between the gas phase and the liquid phase is described by Henry's law:

$$c_g = K_H c_L \quad (50)$$

in which c_g (kg m^{-3}) is the concentration of pesticide in the gas phase and K_H (m^3 m^{-3}) is the Henry coefficient, which is calculated by:

$$K_H = \frac{p_{v,s} M}{S_w R T} \quad (51)$$

where $p_{v,s}$ (Pa) is the saturated vapor pressure, M (kg mol^{-1}) is molar mass, S_w (kg m^{-3}) is solubility in water, R (J mol^{-1} K^{-1}) is the molar gas constant, and T (K) is the temperature. PEARL describes the temperature dependence of both $p_{v,s}$, which requires the molar enthalpy of vaporization, ΔH_v (J mol^{-1}), and S_w, which requires the molar enthalpy of dissolution, ΔH_d (J mol^{-1}):

$$p_{v,s} = p_{v,s,r} \exp\left[\frac{-\Delta H_v}{R}\left(\frac{1}{T}-\frac{1}{T_r}\right)\right] \quad (52)$$

and

$$S_w = S_{w,r} \exp\left[\frac{-\Delta H_d}{R}\left(\frac{1}{T}-\frac{1}{T_r}\right)\right] \quad (53)$$

Here, $p_{v,s,r}$ (Pa) is the saturated vapor pressure at reference temperature T_r (K) and $S_{w,r}$ (kg m^{-3}) is the pesticide solubility in water at reference temperature.

The total concentration of pesticide in the equilibrium domain of the soil system (kg m^{-3}) is given by:

$$c_{eq}^* = \varepsilon c_g + \theta c_L + \rho_b X_{eq} \quad (54)$$

where ε (m^3 m^{-3}) is volume fraction of the gas phase, c_g (kg m^{-3}) is concentration of pesticide in the gas phase, θ (m^3 m^{-3}) is volume fraction of the liquid phase, c_L (kg m^{-3}) is concentration of pesticide in the liquid phase, ρ_b (kg m^{-3}) dry bulk density of the soil, and X_{eq} (kg kg^{-1}) is

pesticide mass content in the equilibrium phase. The total concentration of pesticide in the non-equilibrium phase (kg m^{-3}) is given by:

$$c^*_{ne} = \rho_b X_{ne} \tag{55}$$

with X_{ne} (kg kg^{-1}) as the pesticide mass content in the non-equilibrium phase.

Transformation of pesticide in soil

Transformation of pesticides may lead to reaction products (*daughters*) that may show a certain degree of persistence and mobility in soils. For this reason, the formation and behavior of the most important daughters is included in PEARL. The first step in the definition of the reaction scheme is to set up the list of compounds that will be considered. The second step is the definition of the pathways of pesticide transformation. Consider the example shown in Figure 31. The reaction scheme presented in Figure 31 can be represented in matrix notation as shown in

Table 2. This example shows that a compound may transform into various products and that they may be formed from more than one precursor compound.

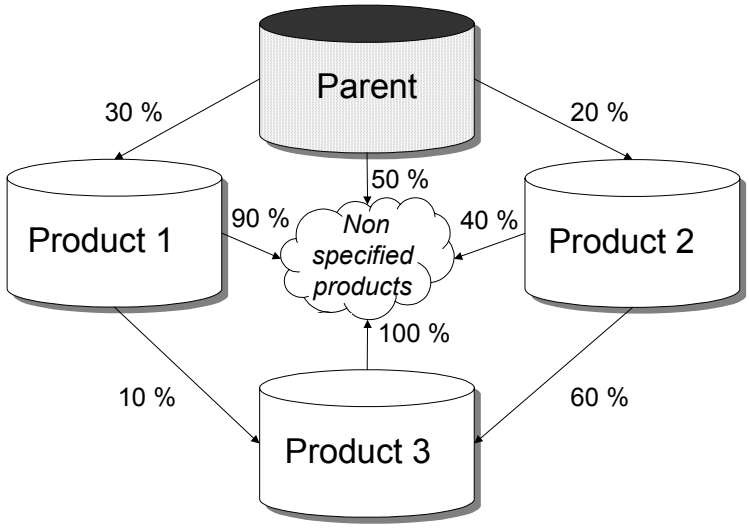


Figure 31 Example of a reaction scheme of a pesticide.

Table 2 Example of a matrix, which represents the reactions between one parent and three reaction products. A value of zero indicates no interaction.

	Parent	Product 1	Product 2	Product 3
Parent	0.0	0.3	0.2	0.0
Product 1	0.0	0.0	0.0	0.1
Product 2	0.0	0.0	0.0	0.6
Product 3	0.0	0.0	0.0	0.0

In PEARL 2.2.2, the rate of transformation of a precursor (*parent*) is described by a first-order rate equation:

$$R_{t,par} = k_{t,par} c^*_{eq,par} \tag{56}$$

in which $R_{t,par}$ (kg m^{-3} d^{-1}) is the rate of transformation of the parent pesticide, $k_{t,par}$ (d^{-1}) is the transformation rate coefficient, and $c^*_{eq,par}$ (kg m^{-3}) is the concentration of the parent pesticide in the equilibrium domain of the soil. *Notice that pesticide residing in the non-equilibrium*

domain is not transformed. The rate of formation of a daughter from a parent, $R_{f,par,dau}$ (kg m^{-3} d^{-1}), is subsequently calculated by:

$$R_{f,par,dau} = \chi_{par,dau} \frac{M_{dau}}{M_{par}} R_{t,par} \tag{57}$$

where $\chi_{par,daugher}$ (-) is the molar fraction of parent transformed to daughter, and M (kg mol^{-1}) is the molar mass.

The rate of pesticide transformation in soil depends on the temperature, soil moisture content and the depth in soil:

$$k_t = f_t f_m f_d k_{t,r} \tag{58}$$

where f_t (-) is the factor for the effect of temperature, f_m (-) is the factor for the effect of soil moisture, f_d (-) is the factor for the effect of depth in soil, and $k_{t,r}$ (d^{-1}) is the rate coefficient at reference conditions, which is calculated from:

$$k_{t,r} = \frac{\ln(2)}{\mathrm{DT}_{50,r}} \tag{59}$$

where $\mathrm{DT}_{50,r}$ (d) is the half-life of the pesticide in the well-moistened plough layer at reference temperature. The effect of temperature on the pesticide transformation rate is described by the Arrhenius equation:

$$f_t = \exp\left[\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right] \tag{60}$$

where E_a (J mol^{-1}) is molar activation energy, R (J mol^{-1} K^{-1}) is the molar gas constant, and T (K) is temperature. The Arrhenius equation is assumed to be valid from 5 to 35 ^{o}C. Above 35 ^{o}C, the factor for the effect of temperature is kept constant. At temperatures below zero, the factor for the effect of temperature is set to zero (Jarvis, 1994). This implies that no pesticide transformation is simulated in frozen soil. The equation for the effect of soil water on transformation reads (Walker, 1974):

$$f_m = \min\left[1, \left(\frac{\theta}{\theta_{fc}}\right)^B\right] \tag{61}$$

where θ (m^3 m^{-3}) is volume fraction of soil water, B (-) is empirical factor for the effect of soil moisture, and the suffix *fc* refers to field capacity. The effect of depth on the rate of transformation in soil is described by a tabular relationship.

In the version of PEARL that is used in GeoPEARL, the transformation in the top horizon (first horizon) can be set dependent on the organic matter content, the clay content and the *p*H of this horizon. The reference half-life, $\mathrm{DT}_{50,r}$, is adjusted according to:

$$\text{if} \begin{cases} DT_{50,plot} < DT_{50,\min} & DT_{50,plot} = DT_{50,\min} \\ DT_{50,\min} < DT_{50,plot} < DT_{50,\max} & DT_{50,plot} = \\ & DT_{50,r} + f_{om}(m_{om} - m_{om.r}) + f_{l}(m_{l} - m_{l,r}) + f_{pH}(p\mathrm{H} - p\mathrm{H}_{r}) \\ DT_{50,plot} > DT_{50,\max} & DT_{50,plot} = DT_{50,\max} \end{cases} \quad (62)$$

where $DT_{50,plot}$ (d) is the plot specific half-life of the pesticide in the well-moistened plough layer at reference temperature, f_{om} (d), f_l (d) and f_{pH} (d) are factors for the effect of organic matter, clay and *p*H, respectively, m_{om} (kg kg^{-3}) is the mass fraction of organic matter, m_l (kg kg^{-3}) is the mass fraction of clay and *p*H is the *p*H of the soil. The suffix *r* refers to the conditions for the reference soil. $DT_{50,min}$ (d) and $DT_{50,max}$ (d) are user-specified minimum and maximum values for the calculated half-live time. The minimum and maximum values are added to prevent the calculation of unrealistic (zero or negative) transformation rates in soils with extreme properties. Such results are due to extrapolation of experimental results. The three factors may act separately, but also in combination. During the simulation the model further corrects for actual soil temperature, soil moisture and depth in the soil profile according to the normal procedure described in Tiktak *et al.* (2000). Figure 32 gives an example of the relationship between *p*H and half-live as introduced with equation 62.

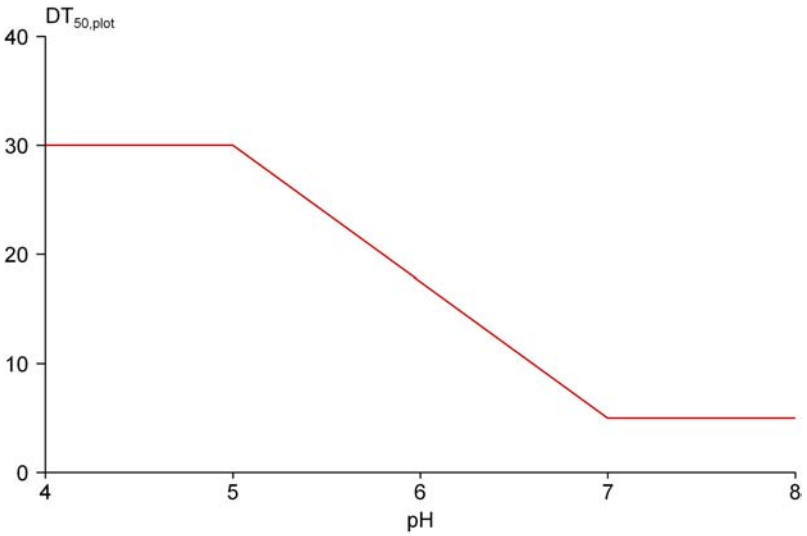


*Figure 32. Half-live as a function of p*H *as introduced with equation 62. In this case, the half-live is dependent on p*H *only and maximum and minimum values have been set.*

In contrast to the sorption process, the dependence of transformation rates on soil properties is described with simple empirical relationships. This rather pragmatic approach has been chosen for several reasons. First, the proposed relationships are compatible with most of the relationships reported in the literature, which are often linear combinations of relationships with basic soil properties; higher order interactions are not often reported. Secondly, the relationships are intended for use in spatially distributed models, which implies that all soil properties should be available in general soil information systems. Organic matter, clay and *p*H are

amongst the most commonly reported soil properties whereas properties like the soil microbial biomass or soil microbial activity, are not.

Pesticide uptake

The uptake of pesticide by plant roots is described by the equation:

$$R_u = R_{u,L} f_u c_L \tag{63}$$

where R_u (kg m^{-3} d^{-1}) is volumic mass rate of pesticide uptake, $R_{u,L}$ (m^3 m^{-3} d^{-1}) is volumic volume rate of water uptake, and f_u (-) is an empirical transpiration stream concentration factor.

Lateral discharge of pesticides

The rate of water discharged by the tile-drainage system is calculated by the hydrological submodel (eqn. (19)). The lateral discharge of pesticides is taken proportional to the water fluxes discharged by the tile-drainage system:

$$R_d = R_{d,L} c_L \tag{64}$$

where R_d (kg m^{-3} d^{-1}) is volumic mass rate of pesticide discharge, and $R_{d,L}$ (m^3 m^{-3} d^{-1}) is volumic volume rate of water discharge. Equation 62 implies that it is assumed that concentration gradients in the lateral direction are negligible (i.e. no diffusion/dispersion).

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